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INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 6 :
C07K 14/705, 14/71, G06F 17/50, 19/00 // 159:00

A1

(11) International Publication Number: WO 99/62955

(43) International Publication Date: 9 December 1999 (09.12.99)

(21) International Application Number: PCT/AU99/00420

(22) International Filing Date: 31 May 1999 (31.05.99)

(30) Priority Data:
PP 3804 29 May 1998 (29.05.98) AU

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(81) Designated States: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published
With international search report.

(54) Title: METHOD OF DESIGNING AGONISTS AND ANTAGONISTS TO EGF RECEPTOR FAMILY

(57) Abstract

The present invention relates to a method of designing compounds able to bind to a molecule of the EGF receptor family and to modulate the activity mediated by the receptor molecule based on the 3-D structure coordinates of the EGF receptor crystal of Figure 6.

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METHOD OF DESIGNING AGONISTS AND ANTAGONISTS TO EGF RECEPTOR FAMILY

Field of the Invention

This invention relates to the field of epidermal growth factor (EGF) receptor structure and EGF receptor/ligand interactions. In particular, it relates to the field of using the EGF receptor structure to select and screen for ligands of the EGF receptor.

Background of the Invention

Epidermal growth factor is a small polypeptide cytokine that stimulates marked proliferation of epithelial tissues and is a member of a larger family of structurally related cytokines such as transforming growth factor α (TGFα), amphiregulin, betacellulin, heparin-binding EGF and some viral gene products. Abnormal EGF family signalling is a characteristic of certain cancers (Soler, C. & Carpenter, G., 1994 In Nicola, N. (ed) "Guidebook to Cytokines and their Receptors", Oxford Univ. Press, Oxford, pp194-197; Walker, F. & Burgess, A. W., 1994, In Nicola, N. (ed) "Guidebook to Cytokines and their Receptors", Oxford Univ. Press, Oxford, pp198-201).

The epidermal growth factor receptor (EGFR) is the cell membrane receptor for EGF (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). The EGFR also binds other ligands that contain amino acid sequences classified as the EGF-like motif. Among these ligands, the three-dimensional structures of EGF and TGFα have been determined by NMR (Montelione, G.T.; Wuthrich, K.; Nice, E.C., Burgess, A.W. and Scheraga, H.A. (1986) *PNAS* 83(22): 8594-8; Campbell, I.D., Cooke, R.M., Baron, M., Harvey, T.S., and Tappin, M.J. (1989) *Prog. Growth Factor Res.* 1, 13-22). Upon binding of the ligand to the extracellular domain, the EGFR undergoes dimerization, which eventually leads to the activation of its cytoplasmic protein tyrosine kinase (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). The EGFR is also known as the ErbB-1 receptor and belongs to the type I family of receptor tyrosine kinases (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). This group also includes the ErbB-2, ErbB-3 and ErbB-4 receptors. The ligand of ErbB-2 is still unknown but it is clear that heregulin binds to ErbB-3 and ErbB-4 (Plowman, G.D., Green, J.M., Calouscou, J.M., Carlton, G.W., Rothwell, V.M., and Buckley, S. (1993) *Nature* 366, 473-475). One of the heregulins is known as neuregulin or NDF and contains an EGF-like sequence that was found to fold into an EGF-like fold by NMR (Nagata, K.,

Kohda, D., Hatanska, H., Ichikawa, S., Matsuda, S., Yamamoto, T., Suzuki, A., and Inagaki, F. (1994) *EMBO J.* 13, 3517-3523 and Jacobson, N.E., Abadl, N., Sliwkowski, M.X., Reilly, D., Skelton, N.J., and Fairbrother, W.J. (1996) *Biochemistry* 36, 3402-3417).

The type II family of receptor tyrosine kinases consists of the insulin receptor (INSR), the insulin-like growth factor I receptor (IGF-1), and the insulin receptor-related receptor (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). Although the type II receptors consist of four chains ($\alpha_2\beta_2$), both the extracellular portions of the receptors from the two families, as well as the tyrosine kinase portions, share significant sequence homology, suggesting a common evolutionary origin (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212, and Bajaj, M., Waterfield, M.D., Schlessinger, J., Taylor, W.R., and Blundell, T. (1987) *Biochim. Biophys. Acta* 916, 220-226).

The 621 amino acid residues of the extracellular domain of the human EGFR (sEGFR) can be subdivided into four domains as follows: L1, S1, L2 and S2, where L and S stand for "large" and "small" domains, respectively (Bajaj, M., Waterfield, M.D., Schlessinger, J., Taylor, W.R., and Blundell, T. (1987) *Biochim. Biophys. Acta* 916, 220-226, see Fig. 2). The L1 and L2 domains are homologous, as are the S1 and S2 domains.

Ligand-induced dimerization was first reported for the EGF receptor (Schlessinger, J. (1980) *Trends Biochem Sci* 13, 443-447) and now is widely accepted as a general mechanism for the transmission of growth stimulatory signals across the cell membrane. Although many biochemical experiments have been performed to reveal the molecular mechanism of receptor dimerization (Lemmon, M.A., Bu, Z., Ladbury, J.E., Zhou, M., Pinchasi, D., Lax, L., Engelman, D.M., and Schlessinger, J. (1997) *EMBO J.* 16, 281-294 and Tzabar, E., Pinkas-Kramarski, R., Moyer, J.D., Klapper, D.N., Alroy, L., Levkowitz, G., Shelly, M., Henis, S., Eisenstein, M., Ratzkin, B.J., Sela, M., Andrews, G.C., and Yarden, Y. (1997) *EMBO J.* 16, 4938-4950 and Lax, L., Mitra, A.K., Ravern, C., Hurwitz, D.R., Rubinstein, M., Ullrich, A., Stroud, R.M., and Schlessinger, J. (1991), *J. Biol. Chem.* 266, 13828-13833), the molecular mechanism by which monomeric ligands induce dimerization is still unknown for members of the EGFR family. Single particle averaging of electron microscopic images suggests that the overall shape of the sEGFR is four-lobed and doughnut-like (Lax, L., Mitra, A.K., Ravern, C., Hurwitz, D.R., Rubinstein, M., Ullrich, A., Stroud, R.M., and Schlessinger, J. (1991), *J. Biol.*

Chem. 266, 13828-13833). Small angle x-ray scattering also indicates that the sEGFR is a flattened sphere with long diameters of 110 Å and a short diameter of 20 Å (Lemmon, M.A., Bu, Z., Ladbury, J.E., Zhou, M., Pinchasi, D., Lax, L., Engelman, D.M., and Schlessinger, J. (1997) *EMBO J.* 16, 281-294). The crystallization of sEGFR in complex with EGF has been published (Günther, N., Betzel, C., and Weber, W. (1990) *J. Biol. Chem.* 265, 22082-22085; Degenhardt M., Weber W., Eschenburg S., Dierks K., Funari SS., Rapp G. and Betzel C. (1998) *Acta Crystallogr, D Biol. Crystallogr.* 54:999-1001), but the structure has not yet been reported, despite a decade of effort by many groups.

One EGF receptor ligand, TGF-α has been observed to be overproduced in keratinocyte cells which are subject to psoriasis (Turbitt, M.L. et al., 1990, *J. Invest. Dermatol.* 95(2), 229-232; Higashimyama, M. et al., 1991, *J. Dermatol.*, 18(2), 117-119; Elder, J.T. et al, 1990, 94(1), 19-25). The overproduction of at least one other EGF receptor ligand, amphiregulin, has also been implicated in psoriasis. (Piepkorn, M. 1996, *Am. J. Dermatopath.*, 18(2), 165-171). Molecules that inhibit the EGF receptor have been shown to inhibit the proliferation of both normal keratinocytes (Dvir, A. et al, 1991, *J. Cell Biol.*, 113(4), 857-865) and psoriatic keratinocytes. (Ben-Bassat, H. et al., 1995, *Exp. Dermatol.*, 4(2), 82-88). These findings indicate that EGF receptor antagonists may be useful in the treatment of psoriasis.

Many cancer cells express constitutively active EGFR (Sandgreen, E. P., et al., 1990, Cell, 61:1121-135; Karnes, W. E. J., et al., 1992, Gastroenterology, 102:474-485) or other EGFR family members (Hynes, N. E.,1993, Semin. Cancer Biol. 4:19-26). Elevated levels of activated EGFR occur in bladder, breast, lung and brain tumours (Harris, A. L., et al., 1989, In Furth & Greaves (eds) The Molecular Diagnostics of human cancer. Cold Spring Harbor Lab. Press, CSH, NY, pp353-357). Antibodies to EGFR can inhibit ligand activation of EGFR (Sato, J. D., et al., 1983 Mol. Biol. Med. 1:511-529) and the growth of many epithelial cell lines (Aboud-Pirak E., et al., 1988, J. Natl Cancer Inst. 85:1327-1331). Patients receiving repeated doses of a humanised chimeric anti-EGFR monoclonal antibody (Mab) showed signs of disease stabilization. The large doses required and the cost of production of humanised Mab is likely to limit the application of this type of therapy. These findings indicate that the development of EGF receptor antagonists will be attractive anticancer agents.

Summary of the Invention

The present inventors have now obtained three-dimensional structural information concerning the epidermal growth factor receptor (EGFR). This structural information was obtained by comparative modelling based on the three-dimensional structure of the IGF-1 receptor as described in PCT/AU98/00998. The information presented in the present application can be used to predict the structure of related members of the EGF receptor family, and to develop specific ligands of members of the EGF receptor family for therapeutic applications.

Accordingly, in a first aspect the present invention provides a method of designing a compound which binds to a molecule of the EGF receptor family and modulates an activity mediated by the molecule, which method comprises the step of assessing the stereochemical complementarity between the compound and a topographic region of the molecule, wherein the molecule is characterised by

(i) amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

(ii) one or more subsets of said amino acids related to the coordinates shown in Figure 6 by whole body translations and/or rotations; or

(iii) amino acids present in the amino acid sequence of a member of the EGF receptor family, which form an equivalent three-dimensional structure to that of the receptor site defined by amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

In a preferred embodiment of the first aspect, the topographic region of the molecule is defined by amino acids 1-475 of the EGF receptor, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

In a further preferred embodiment of the first aspect, the topographic region of the molecule is defined by amino acids 313-621 of the EGF receptor, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

The phrase "EGF receptor family" includes, but is not limited to, the EGF receptor, ErbB2, ErbB3 and ErbB4. In general, EGF receptor family

molecules show similar domain arrangements and share significant sequence identity, preferably at least 40% identity.

The EGF receptor molecule defined in the first aspect of the present invention is depicted in Figure 5. The fragment comprising residues 1-475 of the receptor comprises the L1, S1 and L2 domains of the ectodomain of the EGF receptor. At the centre of this structure is a cavity, bounded by all three domains, of sufficient size to accommodate a ligand molecule.

The fragment comprising residues 313-621 comprises the L2 and S2 domains, which are positioned such that they form a "corner" structure. It is envisaged that this corner structure provides a further binding site for ligands of EGF receptor family members.

By "stereochemical complementarity" we mean that the substance or a portion thereof correlates, in the manner of the classic "lock-and-key" visualisation of ligand-receptor interaction, with the cavity in the receptor site.

In a preferred embodiment of the first aspect of the present invention, the method further involves selecting or designing a compound which has portions that match residues positioned on the surface of the receptor site as depicted in Figures 7, 8 and 9. By "match" we mean that the identified portions interact with the surface residues, for example, via hydrogen bonding or by enthalpy-reducing Van der Waals interactions which promote desolvation of the biologically active compound within the site, in such a way that retention of the compound within the cavity is favoured energetically.

In a further preferred embodiment of the first aspect of the present invention, the method includes screening for, or designing, a compound which possesses a stereochemistry and/or geometry which allows it to interact with both the L1 and L2 domains of the receptor site. It is believed that EGFR monomers may dimerise in nature in such a manner that the cavities of each monomer may face each other. Accordingly, the method of the first aspect of the present invention may involve screening for, or designing, a biologically active compound which interacts with the L1 domain of one monomer and the L2 domain of the other monomer.

In a further preferred embodiment of the first aspect of the present invention the compound interacts with a fragment in the region of the L1 domain-S1 domain interface, causing an alteration in the positions of the

domains relative to each other. Preferably, the interaction of the compound causes the L1 and S1 domains to move away from each other. In a further preferred embodiment the compound interacts with the hinge region between the S1 domain and the L2 domain causing an alteration in the positions of these domains relative to each other. In a further preferred embodiment the compound interacts with the β sheet of the L1 domain causing an alteration in the position of the L1 domain relative to the position of the S1 domain or L2 domain.

In a further preferred embodiment, the compound binds to a lower face (according to orientations shown in Figures 3 and 4) containing the second β-sheet of the L1 and/or L2 domains, wherein the structure of the face is characterised by a plurality of solvent-exposed hydrophobic residues. Examples of these hydrophobic residues include Tyr64, Leu66, Tyr89, Tyr93 (see Figure 7), Leu348, Phe380 and Phe412 (see Figure 10).

In a further preferred embodiment the compound interacts with the hinge region between the L2 domain and S2 domains, causing an alteration in the positions of the L1 and L2 domains relative to each other. Preferably, the interaction of the compound causes the L1 and L2 domains to move away from each other.

In a further preferred embodiment the compound interacts with the β sheet of the L2 domain causing an alteration in the position of the L2 domain relative to the position of the L1 domain.

In a further preferred embodiment of the present invention, the stereochemical complementarity is such that the compound has a K_d for the receptor site of less than 10^{-6}M. More preferably, the K_d value is less than 10^{-8}M and more preferably less than 10^{-9}M.

In preferred embodiments of the first aspect of the present invention, the compound is selected or modified from a known compound identified from a data base.

In one embodiment of the first aspect, the compound has the ability to increase an activity mediated by the molecule of the EGF receptor family.

In another embodiment, the compound has the ability to decrease an activity mediated by the molecule of the EGF receptor family. Preferably, the stereochemical interaction between the compound and the receptor site is adapted to prevent the binding of a natural ligand of the molecule of the EGF

receptor family to the receptor site. Preferably, the compound has a K_i of less than 10^{-6}M, more preferably less than 10^{-8}M and more preferably less than 10^{-9}M.

In a second aspect the present invention provides computer-assisted method for identifying potential compounds able to bind to a molecule of the EGF receptor family and to modulate an activity mediated by the molecule, using a programmed computer comprising a processor, an input device, and an output device, comprising the steps of:

(a) inputting into the programmed computer, through the input device, data comprising the atomic coordinates of the EGF receptor molecule as shown in Figure 6, or a subset thereof;

(b) generating, using computer methods, a set of atomic coordinates of a structure that possesses stereochemical complementarity to the atomic coordinates of the EGF receptor site as shown in Figure 6, or a subset thereof, thereby generating a criteria data set;

(c) comparing, using the processor, the criteria data set to a computer database of chemical structures;

(d) selecting from the database, using computer methods, chemical structures which are similar to a portion of said criteria data set; and

(e) outputting, to the output device, the selected chemical structures which are similar to a portion of the criteria data set.

In a preferred embodiment of the second aspect, the method is used to identify potential compounds which have the ability to decrease an activity mediated by the receptor.

In a further preferred embodiment of the second aspect, the method further comprises the step of selecting one or more chemical structures from step (e) which interact with the receptor site of the molecule in a manner which prevents the binding of natural ligands to the receptor site.

In a further preferred embodiment of the second aspect, the method further comprises the step of obtaining a compound with a chemical structure selected in steps (d) and (e), and testing the compound for the ability to decrease an activity mediated by the receptor.

In a further preferred embodiment of the second aspect, the method is used to identify potential compounds which have the ability to increase an activity mediated by the receptor molecule.

In a further preferred embodiment of the second aspect, the method further comprises the step of obtaining a molecule with a chemical structure

selected in steps (d) and (e), and testing the compound for the ability to increase an activity mediated by the receptor molecule.

The present invention also provides a method of screening of a putative compound having the ability to modulate the activity of a molecule of the EGF receptor family, comprising the steps of identifying a putative compound by a method according to the first or second aspects, and testing the compound for the ability to increase or decrease an activity mediated by the molecule. In one embodiment, the test is carried out *in vitro*. Preferably, the *in vitro* test is a high throughput assay. In another embodiment, the test is carried out *in vivo*.

In a third aspect the present invention provides a compound able to bind to a molecule of the EGF receptor family and to modulate an activity mediated by the molecule, the compound being obtained by a method according to the present invention.

In a preferred embodiment of the third aspect, the compound is a mutant ligand of a molecule of the EGF receptor family, where at least one mutation occurs in the region of the ligand which interacts with residues on the surface of the receptor site facing toward the cavity. For example, the residues Arg 41 and Tyr 13 in EGF are conserved in other members of the EGF receptor family of ligands (a Phe residue may be substituted for Tyr 13). Structures of several EGF family members show the two residues to be in close proximity (Groenen, L.C., Nice, E.C., Burgess, A.W., 1994, Growth Factors 11:235-257). This portion of EGF may interact with a hydrophobic portion of the EGF receptor which contains one or more negatively charged residues such as the lower β sheet of the L1 domain. Mutants of EGF which show altered activity may be generated by introducing modifications to Arg 41 or Tyr 13 or other nearby residues. Alternatively, mutants of EGF may be generated by introducing modifications to residues on the opposite side of the ligand which may interact with a second receptor molecule in the unmodified ligand.

In a fourth aspect the present invention provides a compound which possesses stereochemical complementarity to a topographic region of a molecule of the EGF receptor family and modulates an activity mediated by the molecule, wherein the molecule is characterised by

(i) amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

(ii) one or more subsets of said amino acids related to the coordinates shown in Figure 6 by whole body translations and/or rotations; or

(iii) amino acids present in the amino acid sequence of a member of the EGF receptor family, which form an equivalent three-dimensional structure to that of the receptor site defined by amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

with the proviso that the compound is not a naturally occurring ligand of a molecule of the EGF receptor family or a mutant thereof.

By "mutant" we mean a ligand which has been modified by one or more point mutations, insertions of amino acids or deletions of amino acids.

In a preferred embodiment of the fourth aspect, the topographic region of the molecule is defined by amino acids 1-475 of the EGF receptor or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

In a further preferred embodiment of the fourth aspect, the topographic region of the molecule is defined by amino acids 313-621 of the EGF receptor or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

In preferred embodiments of the third and fourth aspects, the stereochemical complementarity between the compound and the receptor site is such that the compound has a K_d for the receptor site of less than 10^{-6}M, more preferably less than 10^{-8}M.

In some embodiments of the third and fourth aspects, the compound increases an activity mediated by the EGF receptor.

In other embodiments of the third and fourth aspects, the compound decreases an activity mediated by the EGF receptor.

In a fifth aspect, the present invention provides a pharmaceutical composition for preventing or treating a disease which would benefit from increased signalling by a molecule of the EGF receptor family, which comprises a compound according to the third or fourth aspects of the present invention and a pharmaceutically acceptable carrier or diluent.

In a sixth aspect, the present invention provides a pharmaceutical composition for preventing or treating a disease associated with signalling by a molecule of the EGF receptor family which comprises a compound

according to the third or fourth aspects of the present invention and a pharmaceutically acceptable carrier or diluent.

In a seventh aspect the present invention provides a method of preventing or treating a disease which would benefit from increased signalling by a molecule of the EGF receptor family which method comprises administering to a subject in need thereof a compound according to the third or fourth aspects of the present invention. Preferably, the disease is selected from wound healing and gastric ulcers.

In an eighth aspect the present invention provides a method of preventing or treating a disease associated with signalling by a molecule of the EGF receptor family which method comprises administering to a subject in need thereof a compound according to the third or fourth aspects of the present invention. Preferably, the disease is selected from psoriasis and tumour states comprising but not restricted to cancer of the breast, brain, ovary, cervix, pancreas, lung, head and neck, and melanoma, rhabdomyosarcoma, mesothelioma and glioblastoma.

Throughout this specification, the word "comprise", or variations such as "comprises" or "comprising", will be understood to imply the inclusion of a stated element, integer or step, or group of elements, integers or steps, but not the exclusion of any other element, integer or step, or group of elements, integers or steps.

Brief Description of the Drawings

Figure 1: Sequence alignment of human EGF receptor family proteins with IGF-1 receptor sequences and insulin receptor sequence for the first two domains of the EGF receptor. The alignment of the EGF receptor and the various IGF-1 receptor sequences were used by the MODELLER program to create a model of the EGF receptor domains L1 and S1. Residues which are underlined were used to create additional Cα-Cα restraints for the construction of the EGF receptor model. Disulfide bonds are also indicated by lines between cysteine residues. The modules of the EGF receptor S1 domain are numbered.

Figure 2: Sequence alignment of human EGF receptor family proteins with IGF-1 receptor sequences and insulin receptor sequence for the third and

fourth domains of the EGF receptor. Additional labels and lines are similar to those in figure 1.

Figure 3: Model polypeptide fold of the L1 and S1 domains of the EGF receptor. The L1 is at the left hand side of the structure with the N-terminus facing the front. Cysteine residue sidechains are depicted as sticks.

Figure 4: Model polypeptide fold of the L2 and S2 domains of the EGF receptor. The L2 is at the bottom of the structure with the N-terminus facing the front. Cysteine residue sidechains are depicted as sticks.

Figure 5: Superposition of the two models (of the L1 and S1 domain and of L2 and S2 domains) onto the structure of the first three domains of the IGF-1 receptor. Cysteine residue sidechains are depicted as sticks. Selected residues are shown as spheres and labelled.

Figure 6: Coordinates of the two models of the EGF receptor extracellular domain. The first model consists of the domains L1 and S1. The second model consists of the domains L2 and S2. The coordinates are in relation to a Cartesian set of orthogonal axes. The L1, S1 and L2 domains of the EGF receptor models have been superimposed on the crystal structure of the IGF-1 receptor domains L1, cysteine-rich domain and L2. The final column contains the number 20, 40 or 60, depending on whether the residue containing the atom is judged to be well-modelled, have a moderate possibility of error, or is likely to be inaccurate, respectively.

Figure 7: Part of the model polypeptide fold of the L1 and S1 domains of the EGF receptor. Side chains of residues from the L1 domain which face towards the large cavity (shown in Figure 5) are shown in ball and stick notation and labelled with residue number and the one letter code.

Figure 8: Part of the model polypeptide fold of the L1 and S1 domains of the EGF receptor. Side chains of residues from the S1 domain which face towards the large cavity (shown in Figure 5) are shown in ball and stick notation and labelled using the one letter code.

Figure 9: Part of the model polypeptide fold of the L2 and S2 domains of the EGF receptor. Side chains of residues from the L2 domain which face towards the large cavity (shown in Figure 5) are shown in ball and stick notation and labelled using the one letter code.

Figure 10: Part of the model polypeptide fold of the L2 and S2 domains of the EGF receptor. Solvent exposed residues from the face of the L2 domain containing the large β sheet are shown in ball and stick representation.

Detailed description of Preferred Embodiments of the Invention

The present inventors have developed three dimensional structural information about the EGF receptor to enable a more accurate understanding of how the binding of ligand leads to signal transduction. Such information provides a rational basis for the development of ligands for specific therapeutic applications, something that heretofore could not have been predicted *de novo* from available sequence data.

The precise mechanisms underlying the binding of agonists and antagonists to the EGF receptor are not fully clarified. However, the binding of ligands to the receptor site, preferably with an affinity in the order of 10^{-8}M or higher, is understood to arise from enhanced stereochemical complementarity relative to naturally occurring EGF receptor ligands.

Such stereochemical complementarity, pursuant to the present invention, is characteristic of a molecule that matches intra-site surface residues lining the groove of the receptor site as enumerated by the coordinates set out in Figure 6. The residues lining the groove are depicted in Figures 7, 8 and 9. By "match" we mean that the identified portions interact with the surface residues, for example, via hydrogen bonding or by enthalpy-reducing Van der Waals interactions which promote desolvation of the biologically active compound within the site, in such a way that retention of the biologically active compound within the groove is favoured energetically.

Substances which are complementary to the shape of the receptor site characterised by amino acids positioned at atomic coordinates set out in Figure 6 may be able to bind to the receptor site and, when the binding is sufficiently strong, substantially prohibit binding of the naturally occurring ligands to the site.

It will be appreciated that it is not necessary that the complementarity between ligands and the receptor site extend over all residues lining the groove in order to inhibit binding of the natural ligand. Accordingly, agonists or antagonists which bind to a portion of the residues lining the groove are encompassed by the present invention.

In general, the design of a molecule possessing stereochemical complementarity can be accomplished by means of techniques that optimize, either chemically or geometrically, the "fit" between a molecule and a target receptor. Known techniques of this sort are reviewed by Sheridan and Venkataraghavan, Acc. Chem Res. 1987 20 322; Goodford, J. Med. Chem. 1984 27 557; Beddell, Chem. Soc. Reviews 1985, 279; Hol, Angew. Chem. 1986 25 767 and Verlinde C.L.M.J & Hol, W.G.J. Structure 1994, 2, 577, the respective contents of which are hereby incorporated by reference. See also Blundell et al., Nature 1987 326 347 (drug development based on information regarding receptor structure).

Thus, there are two preferred approaches to designing a molecule, according to the present invention, that complements the shape of the EGF receptor. By the geometric approach, the number of internal degrees of freedom (and the corresponding local minima in the molecular conformation space) is reduced by considering only the geometric (hard-sphere) interactions of two rigid bodies, where one body (the active site) contains "pockets" or "grooves" that form binding sites for the second body (the complementing molecule, as ligand). The second preferred approach entails an assessment of the interaction of respective chemical groups ("probes") with the active site at sample positions within and around the site, resulting in an array of energy values from which three-dimensional contour surfaces at selected energy levels can be generated.

The geometric approach is illustrated by Kuntz et al., J. Mol. Biol. 1982 161 269, the contents of which are hereby incorporated by reference, whose algorithm for ligand design is implemented in a commercial software package distributed by the Regents of the University of California and further described in a document, provided by the distributor, which is entitled "Overview of the DOCK Package, Version 1.0,", the contents of which are hereby incorporated by reference. Pursuant to the Kuntz algorithm, the shape of the cavity represented by the EGF receptor site is defined as a series of overlapping spheres of different radii. One or more extant databases of

crystallographic data, such as the Cambridge Structural Database System maintained by Cambridge University (University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K.) and the Protein Data Bank maintained by Brookhaven National Laboratory (Chemistry Dept. Upton, NY 11973, U.S.A.), is then searched for molecules which approximate the shape thus defined.

Molecules identified in this way, on the basis of geometric parameters, can then be modified to satisfy criteria associated with chemical complementarity, such as hydrogen bonding, ionic interactions and Van der Waals interactions.

The chemical-probe approach to ligand design is described, for example, by Goodford, J. Med. Chem. 1985 28 849, the contents of which are hereby incorporated by reference, and is implemented in several commercial software packages, such as GRID (product of Molecular Discovery Ltd., West Way House, Elms Parade, Oxford OX2 9LL, U.K.). Pursuant to this approach, the chemical prerequisites for a site-complementing molecule are identified at the outset, by probing the active site (as represented via the atomic coordinates shown in Fig. 1) with different chemical probes, e.g., water, a methyl group, an amine nitrogen, a carboxyl oxygen, and a hydroxyl. Favored sites for interaction between the active site and each probe are thus determined, and from the resulting three-dimensional pattern of such sites a putative complementary molecule can be generated.

Programs suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore include: MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB Unity (Tripos Associates, St. Louis, MO).

Programs suitable for pharmacophore selection and design include: DISCO (Abbott Laboratories, Abbott Park, IL), Catalyst (Bio-CAD Corp., Mountain View, CA), and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

Databases of chemical structures are available from a number of sources including Cambridge Crystallographic Data Centre (Cambridge, U.K.) and Chemical Abstracts Service (Columbus, OH).

De novo design programs include Ludi (Biosym Technologies Inc., San Diego, CA), Sybyl (Tripos Associates) and Aladdin (Daylight Chemical Information Systems, Irvine, CA).

Those skilled in the art will recognize that the design of a mimetic may require slight structural alteration or adjustment of a chemical structure designed or identified using the methods of the invention.

The invention may be implemented in hardware or software, or a combination of both. However, preferably, the invention is implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object-oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be compiled or interpreted language.

Each such computer program is preferably stored on a storage medium or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The inventive system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

Compounds designed according to the methods of the present invention may be assessed by a number of *in vitro* and *in vivo* assays of hormone function. For example, the identification of EGF receptor antagonists of may be undertaken using a solid-phase receptor binding assay. Potential antagonists may be screened for their ability to inhibit the binding of europium-labelled EGF receptor ligands to soluble, recombinant EGF receptor in a microplate-based format. Europium is a lanthanide fluorophore, the presence of which can be measured using time-resolved fluorometry. The sensitivity of this assay matches that achieved by radioisotopes.

measurement is rapid and is performed in a microplate format to allow high-sample throughput, and the approach is gaining wide acceptance as the method of choice in the development of screens for receptor agonists/antagonists (see Apell et.al. J. Biomolec. Screening 3:19-27, 1998 : Inglese et. al. Biochemistry 37:2372-2377, 1998).

Binding affinity and inhibitor potency may be measured for candidate inhibitors using biosensor technology.

The EGF receptor antagonists may be tested for their ability to modulate receptor activity using a cell-based assay incorporating a stably transfected, EGF-responsive reporter gene (Souriau, C., Fort, P., Roux, P., Hartley, O., Lefranc, M-P., Weill, M., 1997, Nucleic Acids Res. 25:1585-1590). The assay addresses the ability of EGF to activate the reporter gene in the presence of novel ligands. It offers a rapid (results within 6-8 hours of hormone exposure), high-throughput (assay can be conducted in a 96-well format for automated counting) analysis using an extremely sensitive detection system (chemiluminescence). Once candidate compounds have been identified, their ability to antagonise signal transduction via the EGF-R can be assessed using a number of routine in vitro cellular assays such as inhibition of EGF-mediated cell proliferation. Ultimately, the efficiency of antagonist as a tumour therapeutic may be tested in vitro in animals beating tumour isografts and xenografts as described (Rockwell, P., O'Connor, W.J., King, K., Goldstein, N.I., Zhang, L.M., Stein, C.A., 1997, Proc Natl Acad Sci U S A 94:6523-6528; Prewett, M., Rothman, M., Waksal, H., Feldman, M., Bander, N.H., Hicklin, D.J., 1998 Clin Cancer Res 4:2957-2966).

Tumour growth inhibition assays may be designed around a nude mouse xenograft model using a range of cell lines. The effects of the receptor antagonists and inhibitors may be tested on the growth of subcutaneous tumours.

Comparative modelling

The comparative modelling method exploits the observation that proteins with more than 25% amino acid identity will almost always have a similar protein backbone (Sander, C. And Schneider, R., 1991, Proteins: Structure Function and Genetics, 9, 56-68). In some cases, proteins will have similar backbone structures with a lower proportion of identical amino acids. By aligning the sequence of a (target) protein which is to be modelled with the sequences with known structures (the templates), a model of the protein

can be obtained. Where a region of the target sequence follows the sequences of a template, the backbone of the target is built to follow that of the template. Where the target sequence can not be aligned to a target sequence, the so-called insertion must be constructed by other means (Greer, J., 1991, Meth. Enzym. pp 239-252).

The MODELLER program (Šali, A and Blundell, T.L., 1993, J. Mol. Biol. 234, 779-815) is a semi-automated approach to building models of proteins given the structures of one or more template structures and an alignment between the sequences of the target protein and the templates. Based on the sequence alignment and a set of rules derived from the analysis of sets of aligned structure, the program generates a series of restraints for variables such as Cα-Cα distances, main chain and side chain dihedral angles for the target structure. The restraints are expressed in terms of probability density functions (PDFs). The PDFs are combined to yield an expression for the most probable structure as a function of the variables (Cα-Cα distances etc). The program then attempts to find structures to maximise the value of this function. In effect, the program attempts to minimise a transformed version of this function.

While some comparative modelling approaches involve the explicit building of regions of the model for which there is no sequence alignment with a template, the MODELLER program constructs PDFs for these regions, thus including them in the consideration of constructing a comparative model. It is conceivable that once a comparative model has been constructed using MODELLER than an algorithm to build the structures of these regions is applied.

The MODELLER program was used to build the structures of the extracellular portion of the EGF receptor using the 3D structure of the IGF-1 receptor (as described in PCT/AU98/00998) as a template. The description of the generation of these models is outlined below.

Construction of the alignment

The region of the IGF-1 receptor whose structure is known (Garrett, T.P., McKern, N.M., Lou, M., Frenkel, M.J., Bentley, J.D., Lovrecz, G.O., Elleman, T.C., Cosgrove, L.J., Ward, C.W., 1998 Nature 394:395-399) consists of three domains, the L1 domain, cysteine-rich domain (CRD) and the L2 domain (in order of increasing residue number). The L1 and L2 domains adopt similar folds, each consisting of a single-stranded right-hand β-helix.

The helix contains three β-sheets which make up the left and right sides and the bottom of the β-helix. The top is less regular. This type of β-helix has been dubbed a "breadloaf". The cysteine-rich domain (CRD) consists of eight small modules, each of which has one or two disulfide bonds. The first three modules of the CRD contain two disulfide bonds which have a Cys1-Cys3 and Cys2-Cys4 disulfide pairing arrangement. The next four have a single disulfide bond with a so-called β-finger structure. The eighth module of the CRD contains one disulfide bond but is not a β-finger.

The sequence of the EGF receptor extracellular domain can be divided into four domains, L1, S1, L2 and S2 (in order of increasing residue number) on the basis of internal homology and homology with the insulin receptor family (Ward, C.W., Hoyne, P.A., Flegg, R.H., 1995, Proteins 22:141-153; Bajaj, M., Waterfield, M.D., Schlessinger, J., Taylor, W.R., Blundell, T., 1987, Biochim Biophys Acta 916:220-226). The L1 and L2 domains are similar in sequence to each other and to the L1 and L2 domains in the IGF-1 receptor. The S1 and S2 domains are similar in sequence and also similar to the CRD of the IGF-1 receptor. These three domains contain a large number of cysteine residues, although the S2 domain of the EGF receptor has two less cysteine residues than does the CRD of the IGF-1 receptor and the S1 domain of the EGF receptor.

Two important sequence motifs are found in the EGF receptor sequence which are conserved in other EGF receptor homologues. The first motif is the sequence CXXXXXXW which is found near the end of the sequences of the L1 and L2 domains of the EGF receptor and its homologues where C is cysteine and W is tryptophan. (The motif in the L1 domain of the EGF receptor consists of C133-W140 and in the L2 domain consists of C446-W453.) The second motif is the sequence CW which occurs near the start of the S1 and S2 domains of the EGF receptor (C175-W176 in the S1 domain and C491-W492 in the S2 domain). The two motifs also occur in the insulin receptor family (C120XXXXXXW127 and C175W176 in IGF-1 receptor) in the L1 domain and cysteine-rich domain respectively. In contrast to the EGF receptor and its homologues the first of these two motifs does not occur in the L2 domain of the insulin receptor family. Structurally, the first motif corresponds to part of the L1 domain which allows penetration of the tryptophan residue of the second motif into the β-helix. As the first sequence motif is absent from the L2 domain of the IGF-1 receptor, very little of the

structure of this domain was used as a template in the modelling of the EGF receptor.

Construction of the alignment of L1 and S1

As the L1 domain of the IGF-1 receptor has a defined core, the sequence alignment was manually constructed with a view to placing most of the conserved hydrophobic residues of the EGF receptor such that their side chains point towards the β-helical core. Homologues of the EGF receptor were included in the alignment to assist with the identification of such residues (Figure 1). Other IGF-1 receptor residues whose positions were conserved were the four cysteine residues in the L1 domain and the residues Arg 77, Trp 127, Trp 176 and Gln 182. Two small regions of the IGF-1 receptor were also included in the alignment. The first of these regions includes the sequence Ser 375 - Lys 380 from the L2 domain of the IGF-1 receptor and is used as a template for modelling the EGF receptor residues Asp 51 - Lys 56. Additional flanking residues were also used. Residues Ile 385 - Phe 397 of the IGF-1 receptor were also used as a template to better model the EGF receptor residues Ile 83 - Leu 95 (Figure 1).

The alignment of the S1 domain of the EGF receptor to the cysteine-rich domain of the IGF-1 receptor used the same combination of modules. All of the putative modules of the EGF receptor S1 domain were aligned to part or all of the corresponding module of the CRD of the IGF-1 receptor. The third module of the IGF-1 receptor CRD (Cys 201 - Cys 218) was used as an additional template to the first (Cys 166 - Cys 183) and second (Cys 191 - Cys 207) putative modules of the EGF receptor S1 domain. The residues Cys 230 - Cys 246 of IGF-1 receptor, which include the protein's fifth module, were aligned to the EGF receptor residues Cys 267-Cys 283 (which include the EGF receptor S1 domain's putative sixth module).

Construction of the alignment of L2 and S2

Construction of the alignment of the sequence of the L2 domain of the EGF receptor to the sequence of the L1 domain of the IGF-1 receptor followed similar principles to that of the alignment of the L1 domain of the EGF receptor. The region Ile 385 - Phe 397 of the IGF-1 receptor served as an additional template and its sequence was aligned to Ile 402 - Leu 414 of the EGF receptor (Figure 2).

An analysis of β-finger modules in the IGF-1 receptor, TNF receptor and the laminin-γ structures revealed that these modules could be classified

into three types exhibiting some structural and sequence conservation. Two of the structural types are relevant to the IGF-1 receptor and the EGF receptor. The first type of β-finger is characterised by structural conservation of the C-terminal part of the module and also of the linker region after the module. The signature sequence is C...CXXC where the third cysteine residue is the start of another β-finger module. The second type of β-finger is characterised by structural conservation of the N-terminal portion of the module and also of the linker region after the module. The signature sequence is C...CXXXC where the third cysteine is the start of a module whose disulfide bonding pattern has a Cys 1-Cys 3, Cys 2-Cys 4 arrangement.

Comparison of the sequences of the modules of the IGF-1 receptor CRD with the sequence of the EGF receptor S2 domains suggested that the arrangement of modules in the S2 domain were different from those of the IGF receptor CRD and the EGF receptor S1 domain. The residues of the third module in the CRD of the IGF-1 receptor, Cys 201-Cys 218, could be aligned with the segments of the EGF receptor S2 domain sequence: Cys 482 - Cys 499; Cys 534 - Cys 555 and Cys 596 - Cys 612. These modules are the putative first, fourth and seventh modules of the S2 domain. The residues of the first EGF receptor module were also aligned to residues Cys 152 - Cys 181 of the first module of the IGF-1 receptor CRD. The residues of the fourth module in the CRD of the IGF-1 receptor, Cys 221 - Cys 230, a beta-finger module of the first type described above, could be aligned with the regions of sequence Cys 502 - Cys 511 and Cys 558 - Cys 567. These two regions of the EGF receptor S2 domain are the putative second and fifth modules. By elimination, the regions between the two sets of remaining cysteine residues (the putative third and sixth modules) were assigned as β-finger modules of the second type. These regions of sequence are followed by three residues and then a module containing four cysteine residues. The N-terminal regions of the fifth (Cys 234 - Cys 246) and seventh modules (Cys 277 - Cys 291) of the IGF-1 receptor CRD were both aligned to the N-terminal regions of the two modules (Cys 515 - Cys 531 and Cys 571 - Cys 593).

In the IGF-1 receptor CRD, there is no occurrence of a β-finger module being followed by a module containing four cysteine residues. Thus, the positioning of the fourth module in the EGF receptor S2 model relative to the third module is essentially arbitrary. The same applies to the positioning of

the seventh module relative to the sixth module of the EGF receptor S2 domain model.

Construction of the model

Version 3 of the MODELLER program (Modeler User Guide, October 1996, San Diego Molecular Simulations Inc) was used to build models of the EGF receptor. The various sequences of the IGF-1 receptor and the EGF receptor shown in Figure 1 were used as the alignment for the construction of the model of the L1 and S1 domains of the EGF receptor. The coordinates of each of the IGF-1 receptor sequences (i.e. the templates) shown in Figure 1 were also used as input for the MODELLER program. Additional distance restraints were generated between Cα atoms of selected residues. The restraints were generated as follows. The small IGF-1 receptor templates were superimposed into the structure of the first two domains of the IGF-1 receptor using the Cα atoms of the residues which are aligned in Figure 1. Using the Homology module of the Insight II program (Homology User Guide, October 1995, San Diego BIOSYM/MSI) coordinates were built for the EGF receptor residues which are aligned to the IGF-1 receptor coordinates which are in bold typeface. From these coordinates, distance restraints in the form of Gaussian curves were constructed for pairs of Cα atoms with a distance less than 50Å. The sigma value of the Gaussian curves was set to be 2Å. A MODELLER run was submitted using the alignment in Figure 1. The built models of proteins attempt to satisfy these restraints in addition to the restraints the program derives from the alignment.

The aligned IGF-1 receptor and EGF receptor sequences of Figure 2 were used as the alignment for creating the model of the L2 and S2 domains of the EGF receptor. The coordinates of the each of the IGF-1 receptor sequences shown in Figure 2 were used as the structural templates. Two separate sets of additional restraints were used. The first set were based on the underlined IGF-1 receptor residues which are aligned to EGF receptor residues Cys 482 – Cys 534 (the first module of the S2 domain to the first cysteine of the fourth module). From the coordinates of the Cα atoms of these residues, distance restraints in the form of Gaussian curves were constructed for pairs of Cα atoms with a distance less than 50Å. The second set of additional restraints were based on the Cα atoms of the underlined IGF-1 residues which are aligned to EGF receptor residues Cys 534 – Cys 596 (the fourth module of the S2 domain to the first cysteine of the seventh module).

The signal value of the Gaussian curve used to construct the additional restraints was 1Å.

For both sets of models, the MODELLER program constructed 20 models whose coordinates were perturbed from an initial structure by a random value of maximum distance 4Å. The refinement level used was the 'refine1' option in the MODELLER program.

Most of the insertion regions of the EGF receptor models were constructed using the "loop" routine of version 4 of MODELLER (Modeler User Guide, June 1997, San Diego Molecular Simulations Inc) . Coordinates for each insertion were built using one of the two models obtained in the previous section as a scaffold. The regions of sequence for which coordinates were built in this manner were 1-5, 8-12, 16-23, 46-51, 101-107, 145-148, 184-191, 241-262, 319-328, 522-530, 540-546, 578-600 and 612-621. Coordinates for residues 351-368 and 387-393 were constructed simultaneously due to the proximity of these regions in the model of the L2 domain. For each insertion, 50 models were constructed. In cases where the generated loops with the lowest scores had similar backbone structures, the loop building process was considered to have converged and the coordinates of the loop replaced those of the same residues on the refined model. Where the loop structures did not converge, the structures with the three lowest MODELLER loop scores were evaluated using Procheck (Laskowski RA, MacArthur MW, Moss DS, Thornton JM. (1993). J Appl. Crystallogr 26: 283-291), ProsaII (Hendlich M, Lackner P, Weitckus S, Floeckner H, Froschauer R, Gottsbacher K, Casari G, Sippl MJ. (1990) J Mol Biol 216:167-180.; Sippl MJ. (1993) Proteins 17: 355-362.) and Profiles-3D (Bowie JU, Lüthy R, Eisenberg D. (1991) Science 253:164-170.; Lüthy R, Bowie JU, Eisenberg D. 1992. Nature 356:83-85.). For several of these loops, the one with the second lowest MODELLER score was selected as it had a more favorable Profiles3D and ProsaII plot.

In order to retain certain secondary structures, additional restraints were used in the construction of some of the loops. Restraints with the form of a right-handed half-Gaussian function with a s value of 0.05Å were used to hold selected mainchain N-O distances to 3.0Å or less. The atom pairs for which this additional restraint was added were: Gln 139.N - Gln 184.OE1, Val 268.N - Tyr 261.O, Val 268.O - Tyr 261.N, Ser 506.N - Ser 529, Ile 562.N - His 591.O and Glu 578.N - Val 592.

Structure of the EGF receptor model

The structure of the L1 and S1 domains of the EGF receptor as determined by the modelling described above is shown in Figure 3, while the structure of the L2 and S2 domains is shown in Figure 4. The superposition of these two models onto the structure of the extracellular domains of the IGF-1 receptor is shown in Figure 5.

The coordinates of the EGF receptor domains L1, S1, L2 and S2 are shown in Figure 6.

Figures 7, 8 and 9 show the sidechains of residues of the EGF receptor models which face the large cavity as shown in Figure 5. Figure 10 shows the sidechains of residues of the face of the EGF receptor L2 domain which contains the second beta sheet (the lower face of the L2 domain using the orientation shown in Figure 4).

The structures of the L1 and S1 domains are similar to those of the IGF-1 receptor structure, as expected. There are three major differences in the S1 domain of the EGF receptor model from the structure of the IGF-1 receptor cysteine-rich domain. The first module of the S1 domain is noticeably smaller than that of the IGF-1 receptor CRD. The sixth module (Cys 271 – Cys 283) of the S1 domain is smaller than that of the IGF-1 receptor and occupies less of the region between the L1 and L2 domains. The fifth module (Cys 240 – Cys 267) contains a large insertion which points away from the L1 domain. The eighth module of the EGF receptor S1 domain (Cys 305 – Cys 309) and the linker region (Arg 310 – Val 312) which follows it are similar in structure to the analogous regions of the IGF-1 receptor. Like the IGF-1 receptor, the linker region is postulated to be a hinge region about which the S1 domain and the L2 domain can reorient.

A region of the EGF receptor in the L2 domain which could not be aligned with the IGF-1 receptor includes the residues Trp 386 – Pro 387 which are conserved across the EGF receptor family. This sequence motif is not found in the insulin receptor family and may represent a region of novel structure.

The amino acids 352-367 correspond to a large insertion in the L2 domain of the EGF receptor. The amino acids 351-364 have been identified as the epitope for several antibodies against the EGF receptor (Wu, D.G., Wang, L.H., Sato, G.H., West, K.A., Harris, W.R., Crabb, J.W., Sato, J.D., 1989, J. Biol. Chem. 264:17469-17475). This region forms a loop which sticks out of the

surface is consistent with this region being accessible to antibodies. The structure itself is difficult to model accurately since its sequence does not correspond to any part of the IGF-1 receptor sequence. The position of this insertion is in approximately the same region as where the IGF 1 receptor differs in backbone structure.

The S2 domain model of the EGF receptor adopts a different arrangement of modules and consequently a different shape that of the CRD of the IGF-1 receptor and the S1 domain model of the EGF receptor. The disulfide bond arrangement is the same as that predicted by similarity to the tumour necrosis receptor (Ward, C.W., Hoyne, P.A., Flegg, R.H., 1995, Proteins 22:141-153) and has since been confirmed by mass spectroscopic analyses of proteolytically digested EGF receptor extracellular domain (Abe, Y., Odaka, M., Inagaki, F., Lax, I., Schlessinger, J., Kohda, D., 1998, J. Biol. Chem. 273:11150-11157). The only significant contact of the S2 domain with the L2 domain of the EGF receptor model is the intercalation of Trp 492 into the L2 domain, analogous to that made by Trp 176 in the S1 domain of the EGF receptor and Trp 176 in the CRD of the IGF-1 receptor to their respective L1 domains. Unlike the S1 domain of the EGF receptor, the rest of the S2 domain does not make any contacts with the L2 domain. The S2 domain is rod-like and points out from the L2 domain with a different geometry to the manner in which the S1 domain points out from the L1 domain.

Putative binding sites of the EGF receptor

From the IGF-1 receptor structure and a number of insulin receptor mutants, one of the regions of insulin binding was proposed to the face of the L1 domain which contains the second β-sheet (Garrett, T.P., McKern, N.M., Lou, M., Frenkel, M.J., Bentley, J.D., Lovrecz, G.O., Elleman, T.C., Cosgrove, L.J., Ward, C.W., 1998 Nature 394:395-399). This surface is characterised by a number of hydrophobic residues which point out of the structure and also the presence of a structurally conserved loop. By analogy, we propose that the analogous β sheets of the L1 and L2 are potential binding sites. These sheets contain a number of hydrophobic residues, conserved amongst EGF receptor family members, which point away from the core of the β-helix structure. Residue 45 of a mutant EGF has been cross-linked to the residue Lysine 465 which is in the last strand of the lower β sheet of the L2 domain. (Summerfield, AE et al, J Biol Chem, 1996, 271(33), 19656-19659). Tyrosine 101 has been cross-linked to the N-terminus of EGF (Woltjer, RL et al, PNAS,

1992, 89(16), 7801-7805). This residue is in the portion of sequence which immediately follows a strand in the lower β sheet of L1.

The side chain of asparagine 1 of EGF has been cross-linked to lysine 336 of the EGF receptor (Wu, DG et al, PNAS, 1990, 87(8), 3151-3155). The latter residue is in the N-terminal helix of the L2 domain and points towards the cavity which is formed when the two halves of the EGF receptor are postioned in a similar arrangement to the first three domains of the IGF-1 receptor. Two nearby residues, Asn 328 and Asn 337 are glycosylated. This mutation is in a similar position to the insulin receptor mutant S323L which has aberrent insulin binding.

Several insertional mutants of the EGF receptor extracellular domain were constructed to probe the role of several regions of the receptor (Harte, M.T., Gentry, L.E., 1995, Arch Biochem Biophys 322:378-389). A number of these mutants were not detectably secreted by the cells producing them, suggesting that they did not fold to form stable proteins. Most of these insertions were in positions in the model structure where they would be unable to tolerate an insertion. In contrast, most of the other insertions were in loops or other positions which, according to the model, are able to tolerate insertions. EGF receptor extracellular domain mutants with insertions at residues 162, 169, 174 and 220 bound EGF with a similar affinity to the wild-type EGF receptor extracellular domain but bound TGF-α with a lower affinity. The first of these insertions was located one residue before the last cysteine residue of the L1 domain. The second and third insertions were present in the first module of the EGF receptor S1 domain and the fourth was present in the third module of the S1 domain. All of these positions are on a side of the molecule far removed from the large cavity as shown in Figure 5. EGF receptor mutants with insertions at positions 251 (in the fifth module of the S1 domain) and 575 (in the sixth module of the S2 domain) appeared to bind twice as much ligand as the wild-type receptor. Two insertional mutants which showed reduced EGF receptor binding contained insertions at positions 291 (in the seventh module of the S1 domain) and 474 (one residue before the last cysteine of the L2 domain).

Another EGF receptor mutant which shows altered ligand binding behaviour is the R497K mutant. The site of this mutation in the first module of the S2 domain and faces the side of the L2 domain opposite to that containing residue 465. This mutant binds EGF in a similar fashion as wild-

type receptor but abolishes the high affinity binding site for TGF-α (Moriai, T., Kobrin, M.S., Hope, C., Speck, L., Korc, M., 1994, Proc Natl Acad Sci U S A 91:10217-10221).

On the faces containing the second β-sheet (the lower face according to the orientations shown in Figures 3 and 4) of the L1 and L2 domains are a number of solvent-exposed hydrophobic residues including Tyr 64, Leu 66, Tyr 89, Tyr 93, Leu 348, Phe 380 and Phe 412. According to a survey of protein-protein interfaces, tyrosine, phenylalanine and leucine are more likely to be involved in an interface than on the exterior of a protein complex (Tsai C-J, Lin SL, Wolfson, HJ, Nussinov R (1997) Protein Sci 6: 53-64). Lys 465 is located on the lower face of the L2 domain and Tyr 101 is proximal to the lower face fo the L1 domain and are consistent with the lower faces of the domains having roles in ligand binding.

Strategies for developing EGF receptor ligands

For several signalling systems, ligand analogues which have antagonist properties have been described. These ligand include the human growth hormone (Chen WY, Chen NY, Yun J, Wagner TE, Kopchick JJ (1994) J Biol Chem 269:15892-15897), interleukin-6 (Savino R, Lahm A, Salvati AL, Ciapponi L, Sporeno E, Altamura S, Paonessa G, Toniatti C, Ciliberto G EMBO J 1994 Mar 15;13(6):1357-67) and interleukin-4 (Kruse N, Tony HP, Sebald W (1992) EMBO J 11:3237-3244; Zurawski SM, Vega F Jr, Huyghe B, Zurawski G (1993) EMBO J 12:2663-2670). The function of these unmodified ligands is to bind their receptors and then subsequently recruit a second receptor molecule. The mutations of the ligands mentioned above are in positions which interfere with the binding of the second receptor (de Vos AM, Ultsch M, Kossiakoff AA (1992) Science 255:306-312; Brakenhoff JP, de Hon FD, Fontaine V, ten Boekel E, Schooltink H, Rose-John S, Heinrich PC, Content J, Aarden LA (1994) J Biol Chem 269:86-93; Davis ID, Treutlein HR, Friedrich K, Burgess AW (1995) Growth Factors 12:69-83).

To date, no analogues of EGF receptor ligands have been found which are purely antagonistic. Whether EGF and its homologues have sites of binding for two receptor molecules, like the proteins described above, has not been shown. Analysis of 1H NMR transferred nuclear Overhauser enhancement data for titration of TGF-α with the extracellular domain of the EGF receptor indicates that most parts of the ligand are in contact with the receptor upon binding (McInnes C, Hoyt DW, Harkins RN, Pagila RN,

Debanne MT, O'Connor-McCourt M, Sykes BD (1996) J Biol Chem 271:32204-32211). However, the concentrations used in the experiment were such that the dominant receptor species was the ligand-receptor complex with 2:2 stiochiometry. However, even if the ligands of the EGF receptor are buried in the cleft formed by the first three domains of the receptor, it is difficult to envisage that such binding will lead to contact with most of the bound ligand when only one receptor binds the ligand. In an alternative scheme, at least two separate faces on EGF are required to bind into the large cleft of a single EGF receptor molecule which enacts a conformational change in the receptor which then allows it to dimerise. An antagonist may bind to the first binding site of the receptor and not the second, thus preventing dimerisation and subsequent signalling of the receptor. Thus, delineation of the parts of the ligand involved in the (putative) primary and secondary binding faces would greatly assist antagonist design.

Using the EGF receptor model and the known structures of EGF receptor ligands, it may be possible to construct a model, or a partial model, of ligand binding which could suggest which parts of bound ligand are involved in binding to the first and second EGF receptors of the ligand-receptor complex. There are several computer programs that can assist with the construction of such models. Programs such as Quilt (Lijnzaad P, Argos P (1997) Proteins 28:333-343 ; Lijnzaad P, Berendsen HJ, Argos P (1996) Proteins 26:192-203; Lijnzaad P, Berendsen HJ, Argos P 1996 Proteins 25:389-397) can be used to suggest sites on proteins involved in interactions with other proteins. Possible structures of protein complexes can be obtained by programs such as FT-DOCK (Gabb HA, Jackson RM, Sternberg MJ (1997) J Mol Biol 272:106-120) and GRAMM (Vakser IA (1996) Biopolymers 39:455-464; Katchalski-Katzir E, Shariv I, Eisenstein M, Friesem AA, Aflalo C, Vakser IA (1992) Proc Natl Acad Sci U S A 89:2195-2199). The calculation of electrostatic potentials from the Poisson-Boltzmann equation has been used to investigate complexes made up of cytokines and growth factors and their receptors (Demchuk E, Mueller T, Oschkinat H, Sebald W, Wade RC (1994) Protein Sci 3:920-935) and may guide the construction of model complexes. The construction of models will suggest regions of the EGF receptor ligands which may be involved in receptor binding. With the model and supporting experiments, it is envisaged that mutants of EGF and TGF-α will be constructed which are potential antagonists.

The majority of targets for drugs which have made use of structural information are enzymes. One advantage of enzymes over other types of proteins is the presence of substrate-binding clefts whose normal function is to bind small molecule substrates or short lengths of peptides. In contrast, few small molecule inhibitors have been developed which inhibit protein-protein interactions.

Desolvation of protein surfaces appears to be an important factor in the formation of a protein-protein complex. Since, unlike the substrate-binding clefts of enzymes, protein-binding surfaces tend to be much less concave, a bound small molecule is unlikely to provide enough desolvation to enable tight binding. The lower surfaces of the L1 and L2 domains, which have been suggested to be involved in ligand binding, contain hydrophobic regions which suggest that they need to be buried for strong binding of a molecule to these surfaces to occur. We envisage that cyclic molecules, including cyclic peptides, may be able to bind to such surfaces. Hydrophobic functional groups may be chosen which, when bound to the hydrophobic regions of the relevent face, desolvate regions of the protein. Some of the functional groups which interact with the protein will be polar or charged to make favourable electrostatic interactions. Other parts in the cyclic molecule may be polar or charged to increase the aqueous solubility of the molecule. Cyclic molecules also have the advantages of having few possible conformations when unbound, providing a lower loss of entropy upon binding and thus greater binding as compared to a non-cyclic analogue. A degree of flexibility would exist and would allow the molecule to alter its conformation to better accommodate the protein it is binding to.

Algorithms such as LUDI (Bohm HJ (1992) J Comput Aided Mol Des, 6: 593-606) can be used to search for functional groups and molecular moieties which may interact with a surface of the EGF receptor model. Algorithms such as CLIX (Lawrence MC, Davis PC (1992) Proteins 12:31-41) or DOCK (Kuntz ID, Blaney JM, Oatley SJ, Langridge R, Ferrin TE (1982) J Mol Biol 161:269-88) can be used to search a database of molecular structures for those which have shape and/or chemical complementarity to the EGF receptor. Computational combinatorial design algorithms (Miranker A, Karplus M Proteins (1991) 11:29-34; Eisen MB, Wiley DC, Karplus M, Hubbard RE; Caflisch A (1994) Proteins 19:199-221) can also be tried. In one instance, a combinatorial approach has been used to design peptides to

inhibit the interaction of the proteins Ras and Raf (Zeng, J, et al, Protein Engineering, to be published).

We envisage that as an alternative to a cyclic molecule, a small protein could be used as a scaffold for placing amino acids that will interact with the EGF receptor. At least one small protein (potato carboxypeptidase inhibitor) with a fold different to that of EGF receptor ligands has been identified which is a weak EGF antagonist (Blanco-Aparicio C, Molina MA, Fernandez-Salas E, Frazier ML, Mas JM, Querol E, Aviles FX, de Llorens R (1998) J Biol Chem 273:12370-12377). The use of a structural scaffold for proteins with diverse functions has been observed in Nature (Lin SL, Nussinov R 1995 Nat Struct Biol 2:835-837). Other molecular scaffolds such as dendrimers may also be considered which can be used to present the functional groups which will tightly interact with the EGF receptor.

At least two, non-exclusive modes of action can be envisaged. The first mode involves a molecule competing for binding sites with one of the EGF receptor's natural ligands. Most likely, the molecule will prevent the receptor dimerisation which is required for activation of the EGF receptor, thus acting as an antagonist. We do not rule out the possiblity that the binding may be activating and the molecule acts as an agonist. The second potential mode of action is for the molecule to bind to a site on the EGF receptor which is not necessarily a ligand binding site. Such a molecule may be physically large enough to hinder physical access of a second receptor to the receptor which binds the molecule in question. This would hinder dimerisation and subsequent activation of the receptor. If the molecule is sufficiently "sticky", it may attract a second EGF receptor and induce dimerisation, thereby acting as an agonist rather than an antagonist.

It will be appreciated by persons skilled in the art that numerous variations and/or modifications may be made to the invention as shown in the specific embodiments without departing from the spirit or scope of the invention as broadly described. The present embodiments are, therefore, to be considered in all respects as illustrative and not restrictive.

Claims:

1. A method of designing a compound which binds to a molecule of the EGF receptor family and modulates an activity mediated by the molecule, which method comprises the step of assessing the stereochemical complementarity between the compound and a topographic region of the molecule, wherein the molecule is characterised by

(i) amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

(ii) one or more subsets of said amino acids related to the coordinates shown in Figure 6 by whole body translations and/or rotations; or

(iii) amino acids present in the amino acid sequence of a member of the EGF receptor family, which form an equivalent three-dimensional structure to that of the receptor site defined by amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

2. A method as claimed in claim 1 in which the topographic region of the molecule is defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

3. A method as claimed in claim 1 in which the topographic region of the molecule is defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

4. A method as claimed in any one of claims 1 to 3 in which the compound is designed so as to complement the structure of a topographic region of the molecule as depicted in Figure 5.

5. A method as claimed in any one of claims 1 to 4, in which the compound has structural regions able to make close contact with amino acid residues at the surface of the molecule lining the groove as depicted in Figure 7, Figure 8 or Figure 9.

6. A method as claimed in any one of claims 1 to 5, in which the compound has a stereochemistry such that it can interact with both the L1 and L2 domains of the molecule.

7. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the region of the L1 domain-S1 domain interface, causing an alteration in the positions of the L1 and S1 domains relative to each other.

8. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the hinge region between the L2 domain and the S1 domain causing an alteration in the positions of the L2 and S1 domains relative to each other.

9. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the β-sheet of the L1 domain causing an alteration in the position of the L1 domain relative to the position of the S1 domain or the L2 domain.

10. A method as claimed in any one of claims 1 to 5 in which the compound has a stereochemistry such that it can interact with both the L2 and S2 domains of the molecule.

11. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the hinge region between the L2 domain and the S2 domains causing an alteration in the positions of the L1 and L2 domains relative to each other.

12. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the β-sheet of the L2 domain causing an alteration in the position of the L2 domain relative to the position of the S2 domain.

13. A method as claimed in any one of claims 1 to 5, in which the compound binds to a lower face containing the second β-sheet of the L1 and/or L2 domains, wherein the structure of the face is characterised by a plurality of solvent-exposed hydrophobic residues.

14. A method according to claim 13, in which the hydrophobic residues include:

(i) Tyr64, Leu66, Tyr89, Tyr93; and/or

(ii) Leu348, Phe380 and Phe412.

15. A method as claimed in anyone of claims 1 to 14, in which the stereochemical complementarity between the compound and the receptor site is such that the compound has a K_d for the receptor site of less than 10^{-6}M.

16. A method as claimed in claim 15 in which the K_d is less than 10^{-8}M.

17. A method as claimed in any one of claims 1 to 16 in which the compound is selected or modified from a known compound identified from a data base.

18. A method according to any one of claims 1 to 17, in which the compound has the ability to increase an activity mediated by a molecule of the EGF receptor family.

19. A method according to any one of claims 1 to 18, in which the compound has the ability to decrease an activity mediated by a molecule of the EGF receptor family.

20. A method according to claim 19, in which the stereochemical interaction between the compound and the molecule is adapted to prevent the binding of a natural ligand of the receptor molecule to the receptor site.

21. A method according to claim 19 or claim 20, in which the compound has a K_i of less than 10^{-6}M.

22. A method according to claim 21, in which the compound has a K_i of less than 10^{-8}M.

23. A method according to claim 22, in which the compound has a K_i of less than 10^{-9}M.

24. A computer-assisted method for identifying potential compounds able to bind to a molecule of the EGF receptor family and to modulate an activity mediated by the molecule, using a programmed computer comprising a processor, an input device, and an output device, comprising the steps of:

(a) inputting into the programmed computer, through the input device, data comprising the atomic coordinates of the EGF receptor molecule as shown in Figure 6, or a subset thereof;

(b) generating, using computer methods, a set of atomic coordinates of a structure that possesses stereochemical complementarity to the atomic coordinates of a topographic region of the EGF receptor molecule as shown in Figure 6, or a subset thereof, thereby generating a criteria data set;

(c) comparing, using the processor, the criteria data set to a computer database of chemical structures;

(d) selecting from the database, using computer methods, chemical structures which are similar to at least a portion of said criteria data set; and

(e) outputting, to the output device, the selected chemical structures which are similar to a portion of the criteria data set.

25. A computer-assisted method according to claim 24, in which the method is used to identify potential compounds which have the ability to decrease an activity mediated by the molecule.

26. A computer-assisted method according to claim 24 or claim 25, which further comprises the step of selecting one or more chemical structures from step (e) which interact with the molecule in a manner which prevents the binding of natural ligands to the molecule.

27. A computer-assisted method according to any one of claims 24 to 26, which further comprises the step of obtaining a compound with a chemical

structure selected in steps (d) and (e), and testing the compound for the ability to decrease an activity mediated by the molecule.

28. A computer-assisted method according to claim 24, in which the method is used to identify potential compounds which have the ability to increase an activity mediated by the molecule.

29. A computer-assisted method according to claim 28, further comprising the step of obtaining a compound with a chemical structure selected in steps (d) and (e), and testing the compound for the ability to increase an activity mediated by the receptor.

30. A method of screening a putative compound having the ability to modulate the activity of a molecule of the EGF receptor family, comprising the steps of identifying a putative compound by a method according to any one of claims 1 to 29, and testing the compound for the ability to increase or decrease an activity mediated by the molecule.

31. A method according to claim 30, in which the test is carried out *in vitro*.

32. A method according to claim 31, in which the test is a high throughput assay.

33. A method according to claim 30, in which the test is carried out *in vivo*.

34. A method as claimed in any one of claims 1 to 33 in which the molecule of the EGF receptor family is selected from the group consisting of the EGF receptor, ErbB2, ErbB3 and ErbB4.

35. A method as claimed in claim 34 in which the molecule of the EGF receptor family is the EGF receptor.

36. A compound able to bind to a molecule of the EGF receptor family and to modulate an activity mediated by the molecule, the compound being obtained by a method according to any one of claims 1 to 35.

37. A compound which possesses stereochemical complementarity to a topographic region of a molecule of the EGF receptor family and modulates an activity mediated by the molecule, wherein the molecule is characterised by

(i) amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

(ii) one or more subsets of said amino acids related to the coordinates shown in Figure 6 by whole body translations and/or rotations; or

(iii) amino acids present in the amino acid sequence of a member of the EGF receptor family, which form an equivalent three-dimensional structure to that of the receptor site defined by amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

with the proviso that the compound is not a naturally occurring ligand of a molecule of the EGF receptor family or a mutant thereof.

38. A compound as claimed in claim 37 in which the topographic region of the molecule is defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

39. A compound as claimed in claim 37 in which the topographic region of the molecule is defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

40. A compound as claimed in anyone of claims 37 to 39, in which the stereochemical complementarity between the compound and the molecule is such that the compound has a K_d for the receptor site of less than 10^{-6}M.

41. A compound as claimed in claim 40 in which the K_d is less than 10^{-8}M.

42. A compound as claimed in any one of claims 36 to 41, wherein the compound increases an activity mediated by a molecule of the EGF receptor family.

43. A compound as claimed in any one of claims 36 to 41, wherein the compound decreases an activity mediated by a molecule of the EGF receptor family.

44. A compound as claimed in any one of claims 36 to 43 in which the molecule of the EGF receptor family is selected from the group consisting of the EGF receptor, ErbB2, ErbB3 and ErbB4.

45. A compound as claimed in claim 44 in which the molecule of the EGF receptor family is the EGF receptor.

46. A pharmaceutical composition for preventing or treating a disease which would benefit from increased signalling by a molecule of the EGF receptor family, which comprises a compound as claimed in claim 42 and a pharmaceutically acceptable carrier or diluent.

47. A pharmaceutical composition for preventing or treating a disease associated with signalling by a molecule of the EGF receptor family, which comprises a compound as claimed in claim 43 and a pharmaceutically acceptable carrier or diluent.

48. A method of preventing or treating a disease which would benefit from increased signalling by a molecule of the EGF receptor family which method comprises administering to a subject in need thereof a compound as claimed in claim 42.

49. A method according to claim 48 wherein the disease is selected from wound healing and gastric ulcers.

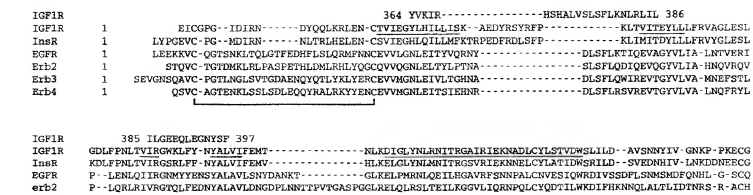
50. A method of preventing or treating a disease associated with signalling by a molecule of the EGF receptor family which method comprises

administering to a subject in need thereof a compound as claimed in claim 43.

51. A method according to claim 50 wherein the disease is selected from psoriasis and tumour states consisting of cancer of the breast, brain, ovary, cervix, pancreas, lung, head and neck, and melanoma, rhabdomyosarcoma, mesothelioma and glioblastoma.

52. A method as claimed in any one of claims 48 to 51 in which the molecule of the EGF receptor family is selected from the group consisting of the EGF receptor, ErbB2, ErbB3 and ErbB4.

53. A method as claimed in claim 52 in which the molecule of the EGF receptor family is the EGF receptor.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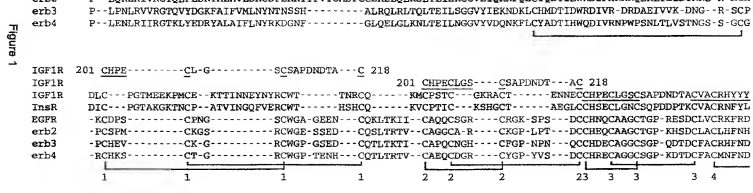
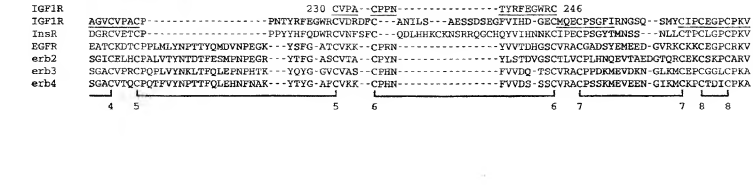
ErbB1 1 EICGPG--IDIRN------DYQQLKRLEN-CTVIEGYLHILLISK--AEDYRSYRFP----------KLTVITEYLLLFRVAGLESL 66
InsR 1 LYPCEVC-PG--MDIRN------NLTRLHELEN-CSVIEGHLQILLMFKTRPEDFRDLSFP----------KLIMITDYLLLFRVYGLESL 71
EGFR 1 LEEKKVC-QGTSNKLTQLGTFEDHFLSLQRMFNNCEVVLGNLEITYVQRNY----------DLSFLKTIQEVAGYVLIA-LNTVERI 75
ErbB2 1 STQVC-TGTDMKLRLPASPETHLDMLRHLYQGCQVVQGNLELTYLPTNA----------SLSFLQDIQEVQGYVLIA-HNQVRQV 73
ErbB3 1 SEVGNSQAVC-PGTLNGLSVTGDAENQYQTLYKLYERCEVVMGNLEIVLTGHNA----------DLSFLQWIREVTGYVLVA-MNEFSTL 78
ErbB4 1 QSVC-AGTENKLSSLSDLEQQYRALRKYYENCEVVMGNLEITSIEHNR----------DLSFLRSVREVTGYVLVA-LNQFRYL 72


IGF1R 385 ILGEEQLEGNYSF 397
ErbB1 GDLFFNLTVIRGWKLFY-NYALVIFEMT----------NLKDIGLYNLRNITRGAIRIEKNADLCYLSTVDWSLILD--AVSNNYIV-GNKP-PKECG 149
InsR KDLFFNLTVIRGSRLFF-NYALVIFEMV----------HLKELGLYNLMNITRGSVRIEKNNELCYLATIDWSRILD--SVEDNHIV-LNKDDNEECG 155
EGFR P--LENLQIIRGNMYYENSYALAVLSNYDANKT----------GLKELPMRNLQEILHGAVRFSNNPALCNVESIQWRDIVSSDFLSNMSMDFQNHL-G-SCQ 164
erb2 P--LQRLRIVRGTQLFEDNYALAVLDNGDPLNNTTPVTGASPGGLRELQLRSLTEILKGGVLIQRNPQLCYQDTILWKDIFHKNNQLALTLIDTNRS-R-ACH 172
erb3 P--LPNLRVVRGTQVYDGKFAIFVMLNYNTNSSH----------ALRQLRLTQLTEILSGGVYIEKNDKLCHMDTIDWRDIVR-DRDAEIVVK-DNG--R-SCP 165
erb4 P--LENLRIIRGTKLYEDRYALAIFLNYRKDGNF----------GLQELGLKNLTEILNGGVYVDQNKFLCYADTIHWQDIVRNPWPSNLTLVSTNGS-S-GCG 162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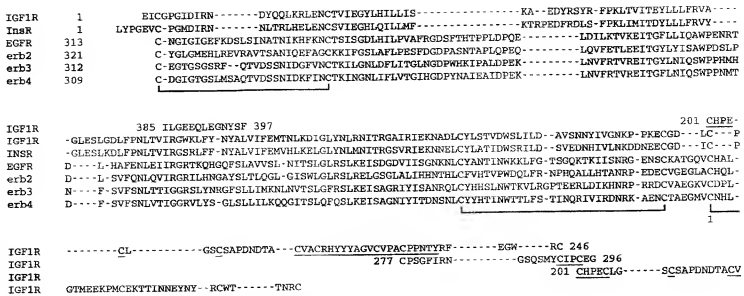
IGF1R 201 CHPECLGS----CSAPDNDT---AC 218
ErbB1 DLC---PGTMEEKPMCE--KTTINNEYNYRCWT------TNRCQ------KMCPSTC---GKRACT------ENNECCHPECLGSCSAPDNDTACVACRHYYY 226
InsR DIC---PGTAKGKTNCP--ATVINGQFVERCWT------HSHCQ------KVCPTIC---KSHGCT------AEGLCCHSECLGNCSQPDDPTKCVACRNFYL 232
EGFR -KCDPS---------CPNG----------SCWGA-GEEN---CQKLTKII--CAQQCSGR----CRGK-SPS---DCCHNQCAAGCTGP-RESDCLVCRKFRD 232
erb2 -PCSPM---------CKGS----------RCWGE-SSED---CQSLTRTV--CAGGCA-R----CKGP-LPT---DCCHEQCAAGCTGP-KHSDCLACLHFNH 239
erb3 -PCHEV---------CK-G----------RCWGP-GSED---CQTLTKTI--CAPQCNGH----CFGP-NPN---QCCHDECAGGCSGP-QDTDCFACRHFND 232
erb4 -RCHKS---------CT-G----------RCWGP-TENH---CQTLTRTV--CAEQCDGR----CYGP-YVS---DCCHRECAGGCSGP-KDTDCFACMNFND 229

IGF1R 230 CVPA--CPPN----------TYREGWRC 246
ErbB1 AGVCVPACP----------PNTYRFEGWRCVDRDFC--ANILS---AESSDSEGFVIHD-GECMQECPSGFIRNGSQ--SMYCIPCEGPCPKV 301
InsR DGRCVETCP----------PPYYHFQDWRCVNFSFC---QDLHHKCKNSRHQGCHQYVIHNNKCIPECPSGYTMNSS---NLLCTPCLGPCPKV 310
EGFR EATCKDTCPPLMLYNPTTYQMDVNPEGK---YSFG-ATCVKK--CPRN----------YVVTDHGSCVRACGADSYEMEED-GVRKCKKCEGPCRKV 312
erb2 SGICELHCPALVTYNTDTFESMPNPEGR---YTFG-ASCVTA--CPYN----------YLSTDVGSCTLVCPLHNQEVTAEDGTQRCEKCSKPCARV 320
erb3 SGACVPRCPQPLVYNKLTFQLEPNPHTK---YQYG-GVCVAS--CPHN----------FVVDQ-TSCVRACPPDKMEVDKN-GLKMCEPCGGLCPKA 311
erb4 SGACVTQCPQTFVYNPTTFQLEHNFNAK---YTYG-APCVKK--CPHN----------FVVDS-SSCVRACPSSKMEVEEN-GIKMCKPCTDICPKA 308

Figure 1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InsR 1 LYPGEVC-PGMDIRN-------NLTRLHELENCSVIEGHLQILLMF----------KTRPEDFRDLS-FPKLIMITDYLLLFRVY---- 66
EGFR 313 C-NGIGIGEFKDSLSINATNIKHFKNCTSISGDLHILPVAFRGDSFTHTPPLDPQE--------LDILKTVKEITGFLLIQAWPENRT 391
erb2 321 C-YGLGMELREVRAVTSANIQEFAGCKKIFGSLAFLPESFDGDPASNTAPLQPEQ--------LQVFETLEEITGYLYISAWPDSLP 399
erb3 312 C-EGTGSGSRF--QTVDSSNIDGFVNCTKILGNLDFLITGLNGDPWHKIPALDPEK--------LNVFRTVREITGYLNIQSWPPHMH 388
erb4 309 C-DGIGTGSLMSAQTVDSSNIDKFINCTKINGNLIFLVTGIHGDPYNAIEAIDPEK--------LNVFRTVREITGFLNIQSWPPNMT 387
IGF1R 385 ILGEEQLEGNYSF 397 201 CHPE- 4
IGF1R -GLESLGDLFPNLTVIRGWKLFY-NYALVIFEMTNLKDIGLYNLRNITRGAIRIEKNADLCYLSTVDWSLILD--AVSNNYIVGNKP-PKECGD---LC---P 153
INSR -GLESLKDLFPNLTVIRGSRLFF-NYALVIFEMVHLKELGLYNLMNITRGSVRIEKNNELCYLATIDWSRILD--SVEDNHIVLNKDDNEECGD---IC---P 159
EGFR D----L-HAFENLEIIRGRTKQHGQFSLAVVSL-NITSLGLRSLKEISDGDVIISGNKNLCYANTINWKKLFG-TSGQKTKIISNRG-ENSCKATGQVCHAL- 485
erb2 D----L-SVFQNLQVIRGRILHNGAYSLTLQGL-GISWLGLRSLRELGSGLALIHHNTHLCFVHTVPWDQLFR-NPHQALLHTANRP-EDECVGEGLACHQL- 493
erb3 N----F-SVFSNLTTIGGRSLYNRGFSLLIMKNLNVTSLGFRSLKEISAGRIYISANRQLCYHHSLNWTKVLRGPTEERLDIKHNRP-RRDCVAEGKVCDPL- 484
erb4 D----F-SVFSNLVTIGGRVLYS-GLSLLILKQQGITSLQFQSLKEISAGNIYITDNSNLCYYHTLNWTTLFS-TINQRIVIRDNRK-AENCTAEGMVCNHL- 481
1

IGF1R --------CL----------GSCSAPDNDTA---CVACRHYYYAGVCVPACPPNTYRF-------EGW-----RC 246
IGF1R 277 CPSGFIRN---------GSQSMYCIPCEG 296
IGF1R 201 CHPECLG------SCSAPDNDTACV 219
IGF1R GTMEEKPMCEKTTINNEYNY--RCWT------TNRC 181
InsR GTAKGKTNCPATVINGQFVE--RCWT------HSHC 187
EGFR --------CS----------PEGCWGP-EPRD---CVSCRNVSRGRECVDKCKLLEGEPREFVENS--------ECIQCHPECLPQA-MNITCTGR-GPDNCI 556
erb2 --------CA----------RGHCWGP-GPTQ---CVNCSQFLRGQECVEECRVLQGLPREYVNAR--------HCLPCHPECQPQN-GSVTCFGP-EADQCV 564
erb3 --------CS----------SGGCWGP-GPGQ---CLSCRNYSRGGVCVTHCNFLNGEPREFAHEA--------ECFSCHPECQPME-GTATCNGS-GSDTCA 555
erb4 --------CS----------SDGCWGP-GPDQ---CLSCRRFSRGRICIESCNLYDGEFREFENGS--------ICVECDPQCEKMEDGLLTCHGP-GPDNCT 553
1 1 1 2 2 3 3 4 4 4 4
IGF1R 201 CHPECLGSCSAPDNDTAC 218
IGF1R 277 CPSGFIRN----------GSQSMYCIPCEG 296
IGF1R ACRHYYYAGVCVPACPPNTYRF----------EGW-----RC 246
EGFR QCAHYIDGPHCVKTCPAGVMGENNTL-VWKYADAGH--------VCHLCHPNCTYGCTGP-GLEGCPTNGPKIPS 621
erb2 ACAHYKDPPFCVARCPSGVKPDLSYMPIWKFPDEEG--------ACQPCPINCTHSCVDL-DDKGCPAEQRASPLT 631
erb3 QCAHFRDGPHCVSSCPHGVLGAKGP--IYKYPDVQN--------ECRPCHENCTQGCKGP-ELQDCLGQTLVLIGKTHLT 624
erb4 KCSHFKDGPNCVEKCPDGLQGANSF--IFKYADPDR--------ECHPCHPNCTQGCNGP-TSHDCIYYPWTGHSTLPQARTP 626
5 5 6 6 7 7 7 7

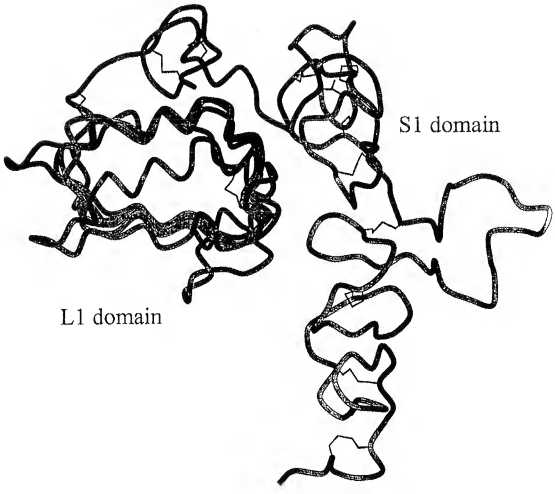

Figure 3

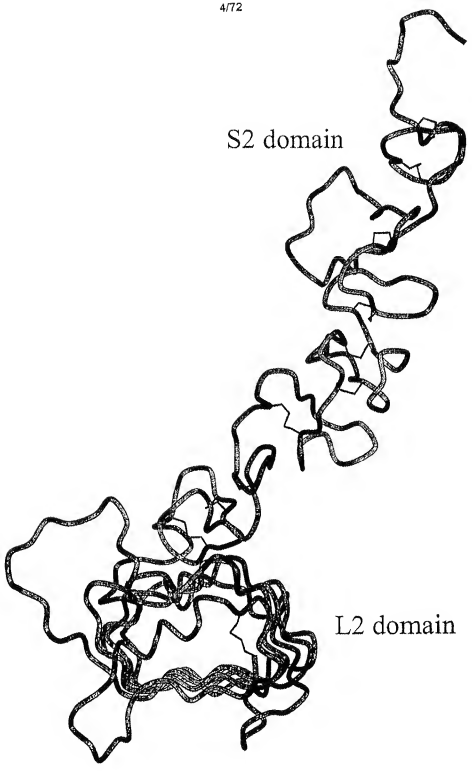

Figure 4

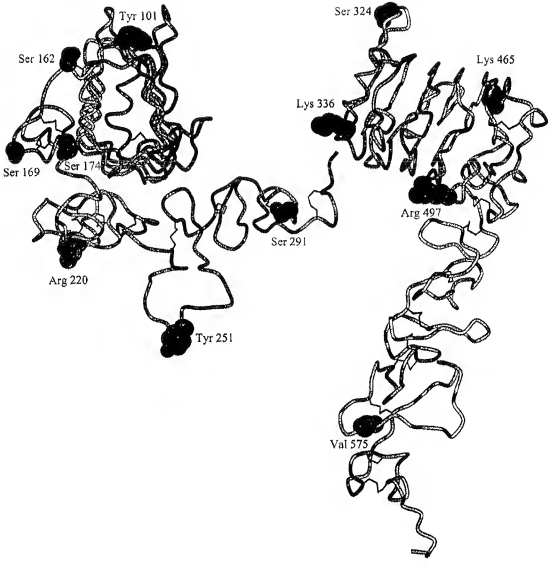
Tyr 101
Ser 162
Ser 169
Ser 174
Arg 220
Tyr 251
Ser 291
Ser 324
Lys 336
Lys 465
Arg 497
Val 575

Figure 5

ATOM	1	N	LEU	1	56.440	23.698	108.904	1.00	60.00
ATOM	2	CA	LEU	1	56.060	23.469	107.493	1.00	60.00
ATOM	3	CB	LEU	1	57.306	23.463	106.595	1.00	60.00
ATOM	4	CG	LEU	1	58.047	24.812	106.566	1.00	60.00
ATOM	5	CD1	LEU	1	59.282	24.747	105.654	1.00	60.00
ATOM	6	CD2	LEU	1	57.097	25.966	106.208	1.00	60.00
ATOM	7	C	LEU	1	55.390	22.146	107.356	1.00	60.00
ATOM	8	O	LEU	1	54.171	22.035	107.470	1.00	60.00
ATOM	9	N	GLU	2	56.181	21.094	107.106	1.00	60.00
ATOM	10	CA	GLU	2	55.627	19.757	106.953	1.00	60.00
ATOM	11	CB	GLU	2	56.680	18.710	106.649	1.00	60.00
ATOM	12	CG	GLU	2	57.348	18.881	105.282	1.00	60.00
ATOM	13	CD	GLU	2	58.367	17.763	105.104	1.00	60.00
ATOM	14	OE1	GLU	2	57.942	16.580	105.009	1.00	60.00
ATOM	15	OE2	GLU	2	59.587	18.080	105.070	1.00	60.00
ATOM	16	C	GLU	2	54.979	19.447	108.254	1.00	60.00
ATOM	17	O	GLU	2	53.886	18.886	108.286	1.00	60.00
ATOM	18	N	GLU	3	55.635	19.811	109.372	1.00	60.00
ATOM	19	CA	GLU	3	55.105	19.488	110.662	1.00	60.00
ATOM	20	CB	GLU	3	55.982	19.975	111.831	1.00	60.00
ATOM	21	CG	GLU	3	57.298	19.207	111.972	1.00	60.00
ATOM	22	CD	GLU	3	58.002	19.710	113.225	1.00	60.00
ATOM	23	OE1	GLU	3	57.458	19.408	114.340	1.00	60.00
ATOM	24	OE2	GLU	3	59.092	20.324	113.085	1.00	60.00
ATOM	25	C	GLU	3	53.771	20.141	110.800	1.00	60.00
ATOM	26	O	GLU	3	52.852	19.560	111.374	1.00	60.00
ATOM	27	N	LYS	4	53.621	21.372	110.272	1.00	60.00
ATOM	28	CA	LYS	4	52.367	22.054	110.404	1.00	60.00
ATOM	29	CB	LYS	4	52.277	23.392	109.663	1.00	60.00
ATOM	30	CG	LYS	4	53.156	24.512	110.204	1.00	60.00
ATOM	31	CD	LYS	4	53.178	25.733	109.282	1.00	60.00
ATOM	32	CE	LYS	4	53.874	26.957	109.876	1.00	60.00
ATOM	33	NZ	LYS	4	53.815	28.084	108.917	1.00	60.00
ATOM	34	C	LYS	4	51.302	21.193	109.810	1.00	60.00
ATOM	35	O	LYS	4	51.578	20.244	109.080	1.00	60.00
ATOM	36	N	LYS	5	50.037	21.508	110.135	1.00	40.00
ATOM	37	CA	LYS	5	48.966	20.748	109.575	1.00	40.00
ATOM	38	CB	LYS	5	47.573	21.255	109.989	1.00	40.00
ATOM	39	CG	LYS	5	47.148	20.806	111.384	1.00	40.00
ATOM	40	CD	LYS	5	47.058	19.284	111.511	1.00	40.00
ATOM	41	CE	LYS	5	46.562	18.804	112.874	1.00	40.00
ATOM	42	NZ	LYS	5	46.275	17.354	112.819	1.00	40.00
ATOM	43	C	LYS	5	49.087	20.925	108.106	1.00	40.00
ATOM	44	O	LYS	5	48.929	19.982	107.333	1.00	40.00
ATOM	45	N	VAL	6	49.383	22.157	107.864	1.00	40.00
ATOM	46	CA	VAL	6	49.512	22.539	106.249	1.00	40.00
ATOM	47	CB	VAL	6	49.637	23.791	105.851	1.00	40.00
ATOM	48	CG1	VAL	6	49.792	23.864	104.325	1.00	40.00
ATOM	49	CG2	VAL	6	48.415	24.543	106.380	1.00	40.00
ATOM	50	C	VAL	6	50.748	21.620	105.810	1.00	40.00
ATOM	51	O	VAL	6	51.656	21.379	106.604	1.00	40.00
ATOM	52	N	CYS	7	50.790	21.227	104.521	1.00	40.00
ATOM	53	CA	CYS	7	51.923	20.529	103.983	1.00	40.00
ATOM	54	CB	CYS	7	51.689	19.021	103.848	1.00	40.00
ATOM	55	SG	CYS	7	51.618	18.187	105.456	1.00	40.00
ATOM	56	C	CYS	7	52.147	21.055	102.605	1.00	40.00
ATOM	57	O	CYS	7	51.319	21.791	102.081	1.00	40.00
ATOM	58	N	GLN	8	53.347	20.797	102.055	1.00	40.00
ATOM	59	CA	GLN	8	53.616	21.165	100.701	1.00	40.00
ATOM	60	CB	GLN	8	54.351	22.508	100.524	1.00	40.00
ATOM	61	CG	GLN	8	53.485	23.727	100.840	1.00	40.00
ATOM	62	CD	GLN	8	54.294	24.975	100.513	1.00	40.00
ATOM	63	OE1	GLN	8	55.306	25.265	101.151	1.00	40.00
ATOM	64	NE2	GLN	8	53.830	25.736	99.482	1.00	40.00
ATOM	65	C	GLN	8	54.512	20.103	100.178	1.00	40.00
ATOM	66	O	GLN	8	55.730	20.163	100.343	1.00	40.00
ATOM	67	N	GLY	9	53.922	19.084	99.537	1.00	40.00
ATOM	68	CA	GLY	9	54.730	18.037	99.000	1.00	40.00
ATOM	69	C	GLY	9	55.099	17.129	100.127	1.00	40.00
ATOM	70	O	GLY	9	55.704	16.080	99.905	1.00	40.00
ATOM	71	N	THR	10	54.744	17.503	101.374	1.00	60.00
ATOM	72	CA	THR	10	55.074	16.629	102.460	1.00	60.00
ATOM	73	CB	THR	10	54.609	17.140	103.793	1.00	60.00
ATOM	74	OG1	THR	10	55.222	18.389	104.079	1.00	60.00
ATOM	75	CG2	THR	10	54.979	16.108	104.873	1.00	60.00
ATOM	76	C	THR	10	54.334	15.371	102.172	1.00	60.00
ATOM	77	O	THR	10	54.902	14.280	102.177	1.00	60.00

Figure 6

ATOM	78	N	SER	11	53.031	15.523	101.874	1.00	60.00
ATOM	79	CA	SER	11	52.244	14.405	101.465	1.00	60.00
ATOM	80	CB	SER	11	50.875	14.310	102.155	1.00	60.00
ATOM	81	OG	SER	11	50.169	13.174	101.676	1.00	60.00
ATOM	82	C	SER	11	52.005	14.661	100.019	1.00	60.00
ATOM	83	O	SER	11	51.261	15.567	99.645	1.00	60.00
ATOM	84	N	ASN	12	52.663	13.866	99.165	1.00	40.00
ATOM	85	CA	ASN	12	52.571	14.073	97.757	1.00	40.00
ATOM	86	CB	ASN	12	53.837	14.744	97.194	1.00	40.00
ATOM	87	CG	ASN	12	53.594	15.173	95.765	1.00	40.00
ATOM	88	OD1	ASN	12	52.470	15.141	95.255	1.00	40.00
ATOM	89	ND2	ASN	12	54.690	15.585	95.063	1.00	40.00
ATOM	90	C	ASN	12	52.500	12.716	97.159	1.00	40.00
ATOM	91	O	ASN	12	51.561	11.957	97.390	1.00	40.00
ATOM	92	N	LYS	13	53.526	12.393	96.359	1.00	40.00
ATOM	93	CA	LYS	13	53.623	11.120	95.726	1.00	40.00
ATOM	94	CB	LYS	13	54.640	11.096	94.569	1.00	40.00
ATOM	95	CG	LYS	13	56.048	11.543	94.970	1.00	40.00
ATOM	96	CD	LYS	13	57.109	11.232	93.914	1.00	40.00
ATOM	97	CE	LYS	13	58.486	11.817	94.235	1.00	40.00
ATOM	98	NZ	LYS	13	58.455	13.291	94.099	1.00	40.00
ATOM	99	C	LYS	13	54.007	10.065	96.701	1.00	40.00
ATOM	100	O	LYS	13	55.183	9.740	96.853	1.00	40.00
ATOM	101	N	LEU	14	53.007	9.495	97.398	1.00	40.00
ATOM	102	CA	LEU	14	53.320	8.352	98.190	1.00	40.00
ATOM	103	CB	LEU	14	52.239	7.967	99.206	1.00	40.00
ATOM	104	CG	LEU	14	52.039	9.020	100.313	1.00	40.00
ATOM	105	CD1	LEU	14	51.544	10.356	99.732	1.00	40.00
ATOM	106	CD2	LEU	14	51.134	8.487	101.436	1.00	40.00
ATOM	107	C	LEU	14	53.498	7.269	97.171	1.00	40.00
ATOM	108	O	LEU	14	52.591	7.186	96.374	1.00	40.00
ATOM	109	N	THR	15	54.469	6.424	97.244	1.00	40.00
ATOM	110	CA	THR	15	54.569	5.441	96.210	1.00	40.00
ATOM	111	CB	THR	15	55.596	5.812	95.123	1.00	40.00
ATOM	112	OG1	THR	15	56.845	5.948	95.665	1.00	40.00
ATOM	113	CG2	THR	15	55.079	7.138	94.488	1.00	40.00
ATOM	114	C	THR	15	55.043	4.163	96.802	1.00	40.00
ATOM	115	O	THR	15	55.565	4.122	97.916	1.00	40.00
ATOM	116	N	GLN	16	54.822	3.059	96.067	1.00	40.00
ATOM	117	CA	GLN	16	55.300	1.792	96.521	1.00	40.00
ATOM	118	CB	GLN	16	54.203	0.712	96.597	1.00	40.00
ATOM	119	CG	GLN	16	54.696	-0.650	97.095	1.00	40.00
ATOM	120	CD	GLN	16	53.502	-1.591	97.151	1.00	40.00
ATOM	121	OE1	GLN	16	52.753	-1.725	96.185	1.00	40.00
ATOM	122	NE2	GLN	16	53.315	-2.259	98.323	1.00	40.00
ATOM	123	C	GLN	16	56.297	1.356	95.502	1.00	40.00
ATOM	124	O	GLN	16	55.946	1.054	94.365	1.00	40.00
ATOM	125	N	LEU	17	57.586	1.354	95.886	1.00	60.00
ATOM	126	CA	LEU	17	58.593	0.969	94.950	1.00	60.00
ATOM	127	CB	LEU	17	60.017	1.078	95.513	1.00	60.00
ATOM	128	CG	LEU	17	60.457	2.521	95.825	1.00	60.00
ATOM	129	CD1	LEU	17	61.887	2.562	96.384	1.00	60.00
ATOM	130	CD2	LEU	17	60.267	3.436	94.605	1.00	60.00
ATOM	131	C	LEU	17	58.338	-0.456	94.601	1.00	60.00
ATOM	132	O	LEU	17	58.466	-0.857	93.446	1.00	60.00
ATOM	133	N	GLY	18	57.948	-1.256	95.608	1.00	60.00
ATOM	134	CA	GLY	18	57.715	-2.643	95.367	1.00	60.00
ATOM	135	C	GLY	18	58.423	-3.369	96.455	1.00	60.00
ATOM	136	O	GLY	18	58.034	-3.308	97.620	1.00	60.00
ATOM	137	N	THR	19	59.502	-4.075	96.088	1.00	60.00
ATOM	138	CA	THR	19	60.271	-4.800	97.051	1.00	60.00
ATOM	139	CB	THR	19	61.451	-5.495	96.444	1.00	60.00
ATOM	140	OG1	THR	19	61.020	-6.425	95.462	1.00	60.00
ATOM	141	CG2	THR	19	62.219	-6.222	97.560	1.00	60.00
ATOM	142	C	THR	19	60.785	-3.785	98.014	1.00	60.00
ATOM	143	O	THR	19	60.907	-4.055	99.209	1.00	60.00
ATOM	144	N	PHE	20	61.089	-2.580	97.497	1.00	60.00
ATOM	145	CA	PHE	20	61.604	-1.517	98.307	1.00	60.00
ATOM	146	CB	PHE	20	61.723	-0.186	97.547	1.00	60.00
ATOM	147	CG	PHE	20	62.734	-0.386	96.468	1.00	60.00
ATOM	148	CD1	PHE	20	64.078	-0.257	96.738	1.00	60.00
ATOM	149	CD2	PHE	20	62.345	-0.708	95.186	1.00	60.00
ATOM	150	CE1	PHE	20	65.015	-0.445	95.750	1.00	60.00
ATOM	151	CE2	PHE	20	63.278	-0.897	94.193	1.00	60.00
ATOM	152	CZ	PHE	20	64.617	-0.765	94.473	1.00	60.00
ATOM	153	C	PHE	20	60.684	-1.332	99.473	1.00	60.00
ATOM	154	O	PHE	20	59.555	-1.819	99.480	1.00	60.00

Figure 6 (continued)

ATOM	155	N	GLU	21	61.184	-0.640	100.514	1.00	60.00
ATOM	156	CA	GLU	21	60.471	-0.440	101.743	1.00	60.00
ATOM	157	CB	GLU	21	61.314	0.262	102.821	1.00	60.00
ATOM	158	CG	GLU	21	62.418	-0.629	103.393	1.00	60.00
ATOM	159	CD	GLU	21	63.461	-0.866	102.306	1.00	60.00
ATOM	160	OE1	GLU	21	63.930	0.172	101.730	1.00	60.00
ATOM	161	OE2	GLU	21	63.798	-2.029	102.033	1.00	60.00
ATOM	162	C	GLU	21	59.239	0.374	101.517	1.00	60.00
ATOM	163	O	GLU	21	58.224	0.142	102.170	1.00	60.00
ATOM	164	N	ASP	22	59.284	1.356	100.600	1.00	60.00
ATOM	165	CA	ASP	22	58.127	2.184	100.414	1.00	60.00
ATOM	166	CB	ASP	22	58.301	3.259	99.327	1.00	60.00
ATOM	167	CG	ASP	22	59.249	4.315	99.878	1.00	60.00
ATOM	168	OD1	ASP	22	59.382	4.443	101.129	1.00	60.00
ATOM	169	OD2	ASP	22	59.909	5.007	99.058	1.00	60.00
ATOM	170	C	ASP	22	56.961	1.325	100.044	1.00	60.00
ATOM	171	O	ASP	22	57.073	0.405	99.235	1.00	60.00
ATOM	172	N	HIS	23	55.803	1.615	100.670	1.00	40.00
ATOM	173	CA	HIS	23	54.586	0.892	100.442	1.00	40.00
ATOM	174	ND1	HIS	23	56.476	-1.838	101.876	1.00	40.00
ATOM	175	NE2	HIS	23	56.905	-2.877	100.017	1.00	40.00
ATOM	176	CE1	HIS	23	57.266	-2.757	101.268	1.00	40.00
ATOM	177	CD2	HIS	23	55.817	-2.148	99.817	1.00	40.00
ATOM	178	CG	HIS	23	56.539	-1.442	100.947	1.00	40.00
ATOM	179	CB	HIS	23	54.466	-0.431	101.225	1.00	40.00
ATOM	180	C	HIS	23	53.501	1.752	101.002	1.00	40.00
ATOM	181	O	HIS	23	53.574	2.979	100.906	1.00	40.00
ATOM	182	N	PHE	24	52.456	1.096	101.537	1.00	40.00
ATOM	183	CA	PHE	24	51.390	1.781	102.206	1.00	40.00
ATOM	184	CB	PHE	24	50.221	0.874	102.641	1.00	40.00
ATOM	185	CG	PHE	24	50.686	-0.097	103.676	1.00	40.00
ATOM	186	CD1	PHE	24	51.333	-1.240	103.312	1.00	40.00
ATOM	187	CD2	PHE	24	50.456	0.154	105.011	1.00	40.00
ATOM	188	CE1	PHE	24	51.755	-2.140	104.269	1.00	40.00
ATOM	189	CE2	PHE	24	50.876	-0.735	105.971	1.00	40.00
ATOM	190	CZ	PHE	24	51.528	-1.885	105.600	1.00	40.00
ATOM	191	C	PHE	24	51.973	2.437	103.414	1.00	40.00
ATOM	192	O	PHE	24	51.413	3.393	103.965	1.00	40.00
ATOM	193	N	LEU	25	53.137	1.940	103.864	1.00	40.00
ATOM	194	CA	LEU	25	53.809	2.441	105.027	1.00	40.00
ATOM	195	CB	LEU	25	55.201	1.807	105.203	1.00	40.00
ATOM	196	CG	LEU	25	55.972	2.301	106.441	1.00	40.00
ATOM	197	CD1	LEU	25	55.274	1.867	107.740	1.00	40.00
ATOM	198	CD2	LEU	25	57.450	1.880	106.387	1.00	40.00
ATOM	199	C	LEU	25	54.004	3.919	104.842	1.00	40.00
ATOM	200	O	LEU	25	53.972	4.680	105.808	1.00	40.00
ATOM	201	N	SER	26	54.210	4.353	103.587	1.00	40.00
ATOM	202	CA	SER	26	54.437	5.732	103.244	1.00	40.00
ATOM	203	CB	SER	26	54.696	5.930	101.740	1.00	40.00
ATOM	204	OG	SER	26	55.877	5.250	101.350	1.00	40.00
ATOM	205	C	SER	26	53.231	6.550	103.603	1.00	40.00
ATOM	206	O	SER	26	53.340	7.745	103.875	1.00	40.00
ATOM	207	N	LEU	27	52.050	5.910	103.620	1.00	40.00
ATOM	208	CA	LEU	27	50.763	6.522	103.842	1.00	40.00
ATOM	209	CB	LEU	27	49.630	5.479	103.835	1.00	40.00
ATOM	210	CG	LEU	27	49.489	4.723	102.500	1.00	40.00
ATOM	211	CD1	LEU	27	48.353	3.693	102.558	1.00	40.00
ATOM	212	CD2	LEU	27	49.347	5.696	101.321	1.00	40.00
ATOM	213	C	LEU	27	50.727	7.196	105.183	1.00	40.00
ATOM	214	O	LEU	27	49.977	8.151	105.379	1.00	40.00
ATOM	215	N	GLN	28	51.536	6.712	106.139	1.00	40.00
ATOM	216	CA	GLN	28	51.542	7.178	107.498	1.00	40.00
ATOM	217	CB	GLN	28	52.603	6.451	108.345	1.00	40.00
ATOM	218	CG	GLN	28	54.035	6.691	107.858	1.00	40.00
ATOM	219	CD	GLN	28	54.993	5.910	108.749	1.00	40.00
ATOM	220	OE1	GLN	28	56.205	5.934	108.543	1.00	40.00
ATOM	221	NE2	GLN	28	54.437	5.195	109.764	1.00	40.00
ATOM	222	C	GLN	28	51.825	8.649	107.578	1.00	40.00
ATOM	223	O	GLN	28	51.263	9.341	108.426	1.00	40.00
ATOM	224	N	ARG	29	52.677	9.183	106.689	1.00	40.00
ATOM	225	CA	ARG	29	53.065	10.561	106.792	1.00	40.00
ATOM	226	CB	ARG	29	54.017	11.010	105.670	1.00	40.00
ATOM	227	CG	ARG	29	55.395	10.355	105.771	1.00	40.00
ATOM	228	CD	ARG	29	56.453	10.977	104.857	1.00	40.00
ATOM	229	NE	ARG	29	56.118	10.623	103.450	1.00	40.00
ATOM	230	CZ	ARG	29	56.967	10.990	102.442	1.00	40.00
ATOM	231	NH1	ARG	29	58.110	11.670	102.726	1.00	40.00

Figure 6 (continued)

ATOM	232	NH2	ARG	29	56.677	10.641	101.152	1.00	40.00
ATOM	233	C	ARG	29	51.854	11.439	106.757	1.00	40.00
ATOM	234	O	ARG	29	51.821	12.487	107.400	1.00	40.00
ATOM	235	N	MET	30	50.818	11.033	106.009	1.00	40.00
ATOM	236	CA	MET	30	49.654	11.851	105.844	1.00	40.00
ATOM	237	CB	MET	30	48.583	11.211	104.944	1.00	40.00
ATOM	238	CG	MET	30	49.009	11.014	103.490	1.00	40.00
ATOM	239	SD	MET	30	47.706	10.321	102.425	1.00	40.00
ATOM	240	CE	MET	30	47.584	8.743	103.316	1.00	40.00
ATOM	241	C	MET	30	48.965	12.114	107.148	1.00	40.00
ATOM	242	O	MET	30	48.518	13.233	107.383	1.00	40.00
ATOM	243	N	PHE	31	48.880	11.112	108.042	1.00	40.00
ATOM	244	CA	PHE	31	48.041	11.271	109.198	1.00	40.00
ATOM	245	CB	PHE	31	48.099	10.049	110.136	1.00	40.00
ATOM	246	CG	PHE	31	47.154	10.272	111.270	1.00	40.00
ATOM	247	CD1	PHE	31	47.538	10.974	112.391	1.00	40.00
ATOM	248	CD2	PHE	31	45.875	9.770	111.210	1.00	40.00
ATOM	249	CE1	PHE	31	46.663	11.173	113.433	1.00	40.00
ATOM	250	CE2	PHE	31	44.995	9.966	112.248	1.00	40.00
ATOM	251	CZ	PHE	31	45.386	10.669	113.360	1.00	40.00
ATOM	252	C	PHE	31	48.418	12.473	110.010	1.00	40.00
ATOM	253	O	PHE	31	47.604	13.375	110.196	1.00	40.00
ATOM	254	N	ASN	32	49.662	12.534	110.513	1.00	40.00
ATOM	255	CA	ASN	32	50.034	13.638	111.352	1.00	40.00
ATOM	256	CB	ASN	32	51.367	13.407	112.087	1.00	40.00
ATOM	257	CG	ASN	32	51.207	12.237	113.045	1.00	40.00
ATOM	258	OD1	ASN	32	50.132	11.639	113.140	1.00	40.00
ATOM	259	ND2	ASN	32	52.294	11.903	113.784	1.00	40.00
ATOM	260	C	ASN	32	50.225	14.877	110.543	1.00	40.00
ATOM	261	O	ASN	32	49.758	15.959	110.898	1.00	40.00
ATOM	262	N	ASN	33	50.899	14.719	109.396	1.00	40.00
ATOM	263	CA	ASN	33	51.396	15.824	108.638	1.00	40.00
ATOM	264	CB	ASN	33	52.295	15.394	107.465	1.00	40.00
ATOM	265	CG	ASN	33	53.634	14.950	108.044	1.00	40.00
ATOM	266	OD1	ASN	33	54.388	14.216	107.417	1.00	40.00
ATOM	267	ND2	ASN	33	53.943	15.436	109.279	1.00	40.00
ATOM	268	C	ASN	33	50.355	16.743	108.089	1.00	40.00
ATOM	269	O	ASN	33	50.562	17.956	108.121	1.00	40.00
ATOM	270	N	CYS	34	49.200	16.267	107.586	1.00	20.00
ATOM	271	CA	CYS	34	48.844	17.318	106.866	1.00	20.00
ATOM	272	CB	CYS	34	48.780	17.152	105.359	1.00	20.00
ATOM	273	SG	CYS	34	50.474	16.567	105.052	1.00	20.00
ATOM	274	C	CYS	34	47.061	17.378	107.054	1.00	20.00
ATOM	275	O	CYS	34	46.342	16.441	106.710	1.00	20.00
ATOM	276	N	GLU	35	46.567	18.492	107.641	1.00	20.00
ATOM	277	CA	GLU	35	45.156	18.756	107.625	1.00	20.00
ATOM	278	CB	GLU	35	44.723	19.956	108.479	1.00	20.00
ATOM	279	CG	GLU	35	43.217	20.215	108.378	1.00	20.00
ATOM	280	CD	GLU	35	42.939	21.643	108.822	1.00	20.00
ATOM	281	OE1	GLU	35	43.355	22.008	109.954	1.00	20.00
ATOM	282	OE2	GLU	35	42.314	22.393	108.025	1.00	20.00
ATOM	283	C	GLU	35	44.854	19.160	106.224	1.00	20.00
ATOM	284	O	GLU	35	43.869	18.732	105.624	1.00	20.00
ATOM	285	N	VAL	36	45.727	20.030	105.674	1.00	20.00
ATOM	286	CA	VAL	36	45.545	20.517	104.342	1.00	20.00
ATOM	287	CB	VAL	36	45.246	21.986	104.291	1.00	20.00
ATOM	288	CG1	VAL	36	45.082	22.406	102.821	1.00	20.00
ATOM	289	CG2	VAL	36	44.012	22.268	105.163	1.00	20.00
ATOM	290	C	VAL	36	46.823	20.314	103.600	1.00	20.00
ATOM	291	O	VAL	36	47.828	20.961	103.884	1.00	20.00
ATOM	292	N	VAL	37	46.821	19.417	102.601	1.00	20.00
ATOM	293	CA	VAL	37	48.027	19.240	101.859	1.00	20.00
ATOM	294	CB	VAL	37	48.137	17.901	101.180	1.00	20.00
ATOM	295	CG1	VAL	37	48.249	16.823	102.273	1.00	20.00
ATOM	296	CG2	VAL	37	46.929	17.691	100.250	1.00	20.00
ATOM	297	C	VAL	37	48.056	20.322	100.830	1.00	20.00
ATOM	298	O	VAL	37	47.191	20.401	99.961	1.00	20.00
ATOM	299	N	LEU	38	49.052	21.222	100.926	1.00	20.00
ATOM	300	CA	LEU	38	49.162	22.282	99.969	1.00	20.00
ATOM	301	CB	LEU	38	49.882	23.531	100.528	1.00	20.00
ATOM	302	CG	LEU	38	49.969	24.782	99.618	1.00	20.00
ATOM	303	CD1	LEU	38	50.711	25.914	100.345	1.00	20.00
ATOM	304	CD2	LEU	38	50.592	24.502	98.238	1.00	20.00
ATOM	305	C	LEU	38	49.954	21.706	98.848	1.00	20.00
ATOM	306	O	LEU	38	51.182	21.679	98.886	1.00	20.00
ATOM	307	N	GLY	39	49.246	21.238	97.807	1.00	20.00
ATOM	308	CA	GLY	39	49.892	20.609	96.695	1.00	20.00

Figure 5 (continued)

ATOM	309	C	GLY	39	48.980	19.511	96.266	1.00	20.00
ATOM	310	O	GLY	39	47.761	19.640	96.353	1.00	20.00
ATOM	311	N	ASN	40	49.540	18.388	95.786	1.00	20.00
ATOM	312	CA	ASN	40	48.656	17.340	95.372	1.00	20.00
ATOM	313	CB	ASN	40	48.718	17.020	93.865	1.00	20.00
ATOM	314	CG	ASN	40	50.125	16.561	93.514	1.00	20.00
ATOM	315	OD1	ASN	40	51.081	17.331	93.595	1.00	20.00
ATOM	316	ND2	ASN	40	50.259	15.270	93.110	1.00	20.00
ATOM	317	C	ASN	40	48.984	16.095	96.124	1.00	20.00
ATOM	318	O	ASN	40	50.032	15.982	96.761	1.00	20.00
ATOM	319	N	LEU	41	48.040	15.135	96.090	1.00	20.00
ATOM	320	CA	LEU	41	48.211	13.866	98.729	1.00	20.00
ATOM	321	CB	LEU	41	47.102	13.532	97.738	1.00	20.00
ATOM	322	CG	LEU	41	47.176	12.079	98.237	1.00	20.00
ATOM	323	CD1	LEU	41	48.519	11.797	98.922	1.00	20.00
ATOM	324	CD2	LEU	41	45.965	11.721	99.113	1.00	20.00
ATOM	325	C	LEU	41	48.146	12.816	95.675	1.00	20.00
ATOM	326	O	LEU	41	47.188	12.755	94.907	1.00	20.00
ATOM	327	N	GLU	42	49.180	11.958	95.595	1.00	20.00
ATOM	328	CA	GLU	42	49.093	10.909	94.627	1.00	20.00
ATOM	329	CB	GLU	42	49.996	11.122	93.398	1.00	20.00
ATOM	330	CG	GLU	42	51.469	11.319	93.740	1.00	20.00
ATOM	331	CD	GLU	42	52.188	11.817	92.496	1.00	20.00
ATOM	332	OE1	GLU	42	51.772	12.880	91.962	1.00	20.00
ATOM	333	OE2	GLU	42	53.162	11.146	92.065	1.00	20.00
ATOM	334	C	GLU	42	49.431	9.626	95.303	1.00	20.00
ATOM	335	O	GLU	42	50.470	9.502	95.950	1.00	20.00
ATOM	336	N	ILE	43	48.523	8.636	95.195	1.00	20.00
ATOM	337	CA	ILE	43	48.778	7.367	95.806	1.00	20.00
ATOM	338	CB	ILE	43	47.667	6.928	96.716	1.00	20.00
ATOM	339	CG2	ILE	43	47.999	5.514	97.270	1.00	20.00
ATOM	340	CG1	ILE	43	47.473	7.939	97.859	1.00	20.00
ATOM	341	CD1	ILE	43	48.669	8.039	98.804	1.00	20.00
ATOM	342	C	ILE	43	48.870	6.372	94.692	1.00	20.00
ATOM	343	O	ILE	43	47.857	5.962	94.131	1.00	20.00
ATOM	344	N	THR	44	50.096	5.931	94.350	1.00	20.00
ATOM	345	CA	THR	44	50.230	5.040	93.234	1.00	20.00
ATOM	346	CB	THR	44	51.275	5.477	92.252	1.00	20.00
ATOM	347	OG1	THR	44	52.554	5.498	92.868	1.00	20.00
ATOM	348	CG2	THR	44	50.919	6.887	91.751	1.00	20.00
ATOM	349	C	THR	44	50.627	3.678	93.719	1.00	20.00
ATOM	350	O	THR	44	51.282	3.535	94.751	1.00	20.00
ATOM	351	N	TYR	45	50.196	2.652	92.951	1.00	20.00
ATOM	352	CA	TYR	45	50.417	1.237	93.111	1.00	20.00
ATOM	353	CB	TYR	45	51.491	0.631	92.188	1.00	20.00
ATOM	354	CG	TYR	45	51.489	-0.836	92.465	1.00	20.00
ATOM	355	CD1	TYR	45	50.437	-1.612	92.032	1.00	20.00
ATOM	356	CD2	TYR	45	52.526	-1.444	93.138	1.00	20.00
ATOM	357	CE1	TYR	45	50.410	-2.964	92.277	1.00	20.00
ATOM	358	CE2	TYR	45	52.505	-2.797	93.385	1.00	20.00
ATOM	359	CZ	TYR	45	51.445	-3.559	92.956	1.00	20.00
ATOM	360	OH	TYR	45	51.417	-4.947	93.208	1.00	20.00
ATOM	361	C	TYR	45	50.743	0.867	94.520	1.00	20.00
ATOM	362	O	TYR	45	51.894	0.594	94.854	1.00	20.00
ATOM	363	N	VAL	46	49.732	0.844	95.407	1.00	20.00
ATOM	364	CA	VAL	46	50.016	0.479	96.764	1.00	20.00
ATOM	365	CB	VAL	46	49.911	1.623	97.730	1.00	20.00
ATOM	366	CG1	VAL	46	50.093	1.074	99.154	1.00	20.00
ATOM	367	CG2	VAL	46	50.944	2.694	97.343	1.00	20.00
ATOM	368	C	VAL	46	49.016	-0.541	97.199	1.00	20.00
ATOM	369	O	VAL	46	47.839	-0.466	96.851	1.00	20.00
ATOM	370	N	GLN	47	49.477	-1.542	97.975	1.00	20.00
ATOM	371	CA	GLN	47	48.569	-2.528	98.482	1.00	20.00
ATOM	372	CB	GLN	47	48.926	-3.970	98.083	1.00	20.00
ATOM	373	CG	GLN	47	48.819	-4.242	96.589	1.00	20.00
ATOM	374	CD	GLN	47	49.200	-5.698	96.348	1.00	20.00
ATOM	375	OE1	GLN	47	48.564	-6.618	96.862	1.00	20.00
ATOM	376	NE2	GLN	47	50.278	-5.916	95.548	1.00	20.00
ATOM	377	C	GLN	47	48.663	-2.463	99.970	1.00	20.00
ATOM	378	O	GLN	47	49.711	-2.745	100.548	1.00	20.00
ATOM	379	N	ARG	48	47.560	-2.076	100.635	1.00	20.00
ATOM	380	CA	ARG	48	47.582	-2.021	102.065	1.00	20.00
ATOM	381	CB	ARG	48	47.560	-0.584	102.621	1.00	20.00
ATOM	382	CG	ARG	48	47.599	-0.497	104.151	1.00	20.00
ATOM	383	CD	ARG	48	47.632	0.938	104.688	1.00	20.00
ATOM	384	NE	ARG	48	47.664	0.865	106.177	1.00	20.00
ATOM	385	CZ	ARG	48	48.202	1.890	106.903	1.00	20.00

Figure 6 (continued)

ATOM	386	NH1	ARG	48	48.705	2.987	106.265	1.00	20.00
ATOM	387	NH2	ARG	48	48.230	1.827	108.266	1.00	20.00
ATOM	388	C	ARG	48	46.342	-2.704	102.530	1.00	20.00
ATOM	389	O	ARG	48	45.269	-2.511	101.962	1.00	20.00
ATOM	390	N	ASN	49	46.464	-3.543	103.574	1.00	40.00
ATOM	391	CA	ASN	49	45.300	-4.204	104.078	1.00	40.00
ATOM	392	CB	ASN	49	45.602	-5.162	105.245	1.00	40.00
ATOM	393	CG	ASN	49	44.344	-5.970	105.616	1.00	40.00
ATOM	394	OD1	ASN	49	43.342	-5.861	104.917	1.00	40.00
ATOM	395	ND2	ASN	49	44.389	-6.842	106.566	1.00	40.00
ATOM	396	C	ASN	49	44.423	-3.124	104.605	1.00	40.00
ATOM	397	O	ASN	49	43.213	-3.115	104.383	1.00	40.00
ATOM	398	N	TYR	50	45.046	-2.163	105.310	1.00	40.00
ATOM	399	CA	TYR	50	44.329	-1.062	105.873	1.00	40.00
ATOM	400	CB	TYR	50	45.065	-0.385	107.039	1.00	40.00
ATOM	401	CG	TYR	50	45.065	-1.389	108.139	1.00	40.00
ATOM	402	CD1	TYR	50	43.945	-1.550	108.921	1.00	40.00
ATOM	403	CD2	TYR	50	46.170	-2.169	108.386	1.00	40.00
ATOM	404	CE1	TYR	50	43.922	-2.473	109.939	1.00	40.00
ATOM	405	CE2	TYR	50	46.155	-3.095	109.403	1.00	40.00
ATOM	406	CZ	TYR	50	45.030	-3.247	110.181	1.00	40.00
ATOM	407	OH	TYR	50	45.011	-4.197	111.224	1.00	40.00
ATOM	408	C	TYR	50	44.098	-0.071	104.787	1.00	40.00
ATOM	409	O	TYR	50	44.522	-0.271	103.650	1.00	40.00
ATOM	410	N	ASP	51	43.384	1.022	105.110	1.00	40.00
ATOM	411	CA	ASP	51	43.064	1.961	104.081	1.00	40.00
ATOM	412	CB	ASP	51	41.852	2.170	103.854	1.00	40.00
ATOM	413	CG	ASP	51	41.629	0.814	103.272	1.00	40.00
ATOM	414	OD1	ASP	51	41.865	-0.089	102.997	1.00	40.00
ATOM	415	OD2	ASP	51	39.787	0.701	103.095	1.00	40.00
ATOM	416	C	ASP	51	43.603	3.307	104.437	1.00	40.00
ATOM	417	O	ASP	51	44.260	3.501	105.458	1.00	40.00
ATOM	418	N	LEU	52	43.326	4.261	103.530	1.00	40.00
ATOM	419	CA	LEU	52	43.698	5.646	103.552	1.00	40.00
ATOM	420	CB	LEU	52	43.336	6.381	102.252	1.00	40.00
ATOM	421	CG	LEU	52	44.104	5.860	101.024	1.00	40.00
ATOM	422	CD1	LEU	52	43.732	4.403	100.706	1.00	40.00
ATOM	423	CD2	LEU	52	43.931	6.799	99.821	1.00	40.00
ATOM	424	C	LEU	52	42.980	6.329	104.672	1.00	40.00
ATOM	425	O	LEU	52	43.418	7.367	105.163	1.00	40.00
ATOM	426	N	SER	53	41.876	5.719	105.136	1.00	40.00
ATOM	427	CA	SER	53	40.953	6.292	106.070	1.00	40.00
ATOM	428	CB	SER	53	39.351	5.261	106.618	1.00	40.00
ATOM	429	OG	SER	53	40.631	4.269	107.373	1.00	40.00
ATOM	430	C	SER	53	41.684	6.865	107.239	1.00	40.00
ATOM	431	O	SER	53	41.186	7.794	107.873	1.00	40.00
ATOM	432	N	PHE	54	42.881	6.349	107.561	1.00	40.00
ATOM	433	CA	PHE	54	43.588	6.840	108.706	1.00	40.00
ATOM	434	CB	PHE	54	44.964	6.180	108.931	1.00	40.00
ATOM	435	CG	PHE	54	45.821	6.394	107.731	1.00	40.00
ATOM	436	CD1	PHE	54	46.628	7.502	107.674	1.00	40.00
ATOM	437	CD2	PHE	54	45.819	5.475	106.709	1.00	40.00
ATOM	438	CE1	PHE	54	47.418	7.686	106.511	1.00	40.00
ATOM	439	CE2	PHE	54	46.605	5.651	105.595	1.00	40.00
ATOM	440	CZ	PHE	54	47.407	6.760	105.494	1.00	40.00
ATOM	441	C	PHE	54	43.779	8.321	108.578	1.00	40.00
ATOM	442	O	PHE	54	43.763	9.023	109.588	1.00	40.00
ATOM	443	N	LEU	55	43.976	8.845	107.352	1.00	40.00
ATOM	444	CA	LEU	55	44.137	10.268	107.216	1.00	40.00
ATOM	445	CB	LEU	55	44.704	10.676	105.847	1.00	40.00
ATOM	446	CG	LEU	55	44.884	12.193	105.681	1.00	40.00
ATOM	447	CD1	LEU	55	45.897	12.750	106.696	1.00	40.00
ATOM	448	CD2	LEU	55	45.243	12.549	104.232	1.00	40.00
ATOM	449	C	LEU	55	42.784	10.895	107.360	1.00	40.00
ATOM	450	O	LEU	55	42.167	11.322	106.384	1.00	40.00
ATOM	451	N	LYS	56	42.295	10.952	108.613	1.00	40.00
ATOM	452	CA	LYS	56	41.021	11.494	108.983	1.00	40.00
ATOM	453	CB	LYS	56	40.684	11.190	110.451	1.00	40.00
ATOM	454	CG	LYS	56	39.337	11.745	110.910	1.00	40.00
ATOM	455	CD	LYS	56	38.977	11.337	112.341	1.00	40.00
ATOM	456	CE	LYS	56	39.847	12.023	113.398	1.00	40.00
ATOM	457	NZ	LYS	56	39.445	11.587	114.764	1.00	40.00
ATOM	458	C	LYS	56	41.024	12.987	108.854	1.00	40.00
ATOM	459	O	LYS	56	40.057	13.582	108.382	1.00	40.00
ATOM	460	N	THR	57	42.138	13.618	109.273	1.00	20.00
ATOM	461	CA	THR	57	42.263	15.045	109.401	1.00	20.00
ATOM	462	CB	THR	57	43.574	15.452	110.004	1.00	20.00

Figure 6 (continued)

ATOM	463	OG1	THR	57	43.716	14.887	111.300	1.00	20.00
ATOM	464	CG2	THR	57	43.618	16.986	110.088	1.00	20.00
ATOM	465	C	THR	57	42.147	15.766	108.095	1.00	20.00
ATOM	466	O	THR	57	41.559	16.845	108.044	1.00	20.00
ATOM	467	N	ILE	58	42.691	15.207	107.001	1.00	20.00
ATOM	468	CA	ILE	58	42.752	15.953	105.774	1.00	20.00
ATOM	469	CB	ILE	58	43.416	15.202	104.603	1.00	20.00
ATOM	470	CG2	ILE	58	42.628	13.911	104.365	1.00	20.00
ATOM	471	CG1	ILE	58	43.605	16.125	103.437	1.00	20.00
ATOM	472	CD1	ILE	58	44.643	15.551	102.377	1.00	20.00
ATOM	473	C	ILE	58	41.407	16.442	105.323	1.00	20.00
ATOM	474	O	ILE	58	40.596	15.695	104.777	1.00	20.00
ATOM	475	N	GLN	59	41.124	17.731	105.614	1.00	20.00
ATOM	476	CA	GLN	59	39.940	18.413	105.171	1.00	20.00
ATOM	477	CB	GLN	59	39.886	19.650	106.016	1.00	20.00
ATOM	478	CG	GLN	59	39.114	19.318	107.433	1.00	20.00
ATOM	479	CD	GLN	59	38.798	20.630	108.139	1.00	20.00
ATOM	480	OE1	GLN	59	37.646	20.908	108.470	1.00	20.00
ATOM	481	NE2	GLN	59	39.846	21.464	108.372	1.00	20.00
ATOM	482	C	GLN	59	40.087	18.883	103.783	1.00	20.00
ATOM	483	O	GLN	59	39.119	18.885	102.994	1.00	20.00
ATOM	484	N	GLU	60	41.302	19.315	103.351	1.00	20.00
ATOM	485	CA	GLU	60	41.406	19.919	102.052	1.00	20.00
ATOM	486	CB	GLU	60	41.582	21.445	102.130	1.00	20.00
ATOM	487	CG	GLU	60	40.426	22.179	102.808	1.00	20.00
ATOM	488	CD	GLU	60	40.902	23.597	103.121	1.00	20.00
ATOM	489	OE1	GLU	60	42.013	23.957	102.650	1.00	20.00
ATOM	490	OE2	GLU	60	40.168	24.323	103.840	1.00	20.00
ATOM	491	C	GLU	60	42.625	19.426	101.339	1.00	20.00
ATOM	492	O	GLU	60	43.535	18.884	101.933	1.00	20.00
ATOM	493	N	VAL	61	42.623	19.617	100.003	1.00	20.00
ATOM	494	CA	VAL	61	43.739	19.371	99.139	1.00	20.00
ATOM	495	CB	VAL	61	43.618	18.104	98.346	1.00	20.00
ATOM	496	CG1	VAL	61	44.815	18.008	97.386	1.00	20.00
ATOM	497	CG2	VAL	61	43.510	16.923	99.325	1.00	20.00
ATOM	498	C	VAL	61	43.663	20.512	98.175	1.00	20.00
ATOM	499	O	VAL	61	42.629	20.706	97.541	1.00	20.00
ATOM	500	N	ALA	62	44.739	21.307	98.028	1.00	20.00
ATOM	501	CA	ALA	62	44.601	22.467	97.194	1.00	20.00
ATOM	502	CB	ALA	62	45.522	23.621	97.628	1.00	20.00
ATOM	503	C	ALA	62	44.949	22.139	95.778	1.00	20.00
ATOM	504	O	ALA	62	45.261	23.037	94.998	1.00	20.00
ATOM	505	N	GLY	63	44.913	20.849	95.400	1.00	20.00
ATOM	506	CA	GLY	63	45.218	20.512	94.039	1.00	20.00
ATOM	507	C	GLY	63	44.232	19.500	93.561	1.00	20.00
ATOM	508	O	GLY	63	43.030	19.748	93.502	1.00	20.00
ATOM	509	N	TYR	64	44.743	18.311	93.190	1.00	20.00
ATOM	510	CA	TYR	64	43.878	17.267	92.734	1.00	20.00
ATOM	511	CB	TYR	64	43.952	17.027	91.216	1.00	20.00
ATOM	512	CG	TYR	64	45.282	16.458	90.869	1.00	20.00
ATOM	513	CD1	TYR	64	46.437	17.086	91.267	1.00	20.00
ATOM	514	CD2	TYR	64	45.375	15.321	90.104	1.00	20.00
ATOM	515	CE1	TYR	64	47.666	16.569	90.923	1.00	20.00
ATOM	516	CE2	TYR	64	46.603	14.803	89.766	1.00	20.00
ATOM	517	CZ	TYR	64	47.754	15.422	90.178	1.00	20.00
ATOM	518	OH	TYR	64	49.014	14.890	89.831	1.00	20.00
ATOM	519	C	TYR	64	44.285	16.029	93.455	1.00	20.00
ATOM	520	O	TYR	64	45.341	15.991	94.083	1.00	20.00
ATOM	521	N	VAL	65	43.422	14.996	93.431	1.00	20.00
ATOM	522	CA	VAL	65	43.773	13.787	94.112	1.00	20.00
ATOM	523	CB	VAL	65	42.806	13.411	95.195	1.00	20.00
ATOM	524	CG1	VAL	65	41.422	13.221	94.564	1.00	20.00
ATOM	525	CG2	VAL	65	43.342	12.159	95.910	1.00	20.00
ATOM	526	C	VAL	65	43.821	12.671	93.113	1.00	20.00
ATOM	527	O	VAL	65	42.893	12.479	92.329	1.00	20.00
ATOM	528	N	LEU	66	44.934	11.906	93.110	1.00	20.00
ATOM	529	CA	LEU	66	45.043	10.791	92.210	1.00	20.00
ATOM	530	CB	LEU	66	46.320	10.774	91.355	1.00	20.00
ATOM	531	CG	LEU	66	46.480	11.929	90.359	1.00	20.00
ATOM	532	CD1	LEU	66	47.728	11.779	89.521	1.00	20.00
ATOM	533	CD2	LEU	66	45.187	12.092	89.499	1.00	20.00
ATOM	534	C	LEU	66	45.142	9.553	93.039	1.00	20.00
ATOM	535	O	LEU	66	45.964	9.471	93.951	1.00	20.00
ATOM	536	N	ILE	67	44.301	8.544	92.747	1.00	20.00
ATOM	537	CA	ILE	67	44.414	7.352	93.528	1.00	20.00
ATOM	538	CB	ILE	67	43.344	7.223	94.576	1.00	20.00
ATOM	539	CG2	ILE	67	41.980	7.108	93.873	1.00	20.00

Figure 6 (continued)

ATOM	540	CG1	ILE	67	43.670	6.062	95.530	1.00	20.00
ATOM	541	CD1	ILE	67	42.805	6.050	96.789	1.00	20.00
ATOM	542	C	ILE	67	44.326	6.154	92.637	1.00	20.00
ATOM	543	O	ILE	67	43.429	6.036	91.809	1.00	20.00
ATOM	544	N	ALA	68	45.306	5.248	92.781	1.00	40.00
ATOM	545	CA	ALA	68	45.292	3.994	92.090	1.00	40.00
ATOM	546	CB	ALA	68	46.147	3.983	90.811	1.00	40.00
ATOM	547	C	ALA	68	45.906	3.023	93.057	1.00	40.00
ATOM	548	O	ALA	68	47.087	3.150	93.373	1.00	40.00
ATOM	549	N	LEU	69	45.135	2.029	93.551	1.00	40.00
ATOM	550	CA	LEU	69	45.680	1.141	94.543	1.00	40.00
ATOM	551	CB	LEU	69	45.501	1.657	95.981	1.00	40.00
ATOM	552	CG	LEU	69	46.280	2.945	96.317	1.00	40.00
ATOM	553	CD1	LEU	69	46.036	3.378	97.774	1.00	40.00
ATOM	554	CD2	LEU	69	47.775	2.793	96.000	1.00	40.00
ATOM	555	C	LEU	69	44.949	-0.160	94.495	1.00	40.00
ATOM	556	O	LEU	69	44.091	-0.367	93.643	1.00	40.00
ATOM	557	N	ASN	70	45.312	-1.065	95.430	1.00	40.00
ATOM	558	CA	ASN	70	44.673	-2.342	95.643	1.00	40.00
ATOM	559	CB	ASN	70	45.584	-3.527	95.195	1.00	40.00
ATOM	560	CG	ASN	70	45.968	-3.425	93.715	1.00	40.00
ATOM	561	OD1	ASN	70	45.513	-2.541	92.992	1.00	40.00
ATOM	562	ND2	ASN	70	46.838	-4.367	93.259	1.00	40.00
ATOM	563	C	ASN	70	44.318	-2.510	96.984	1.00	40.00
ATOM	564	O	ASN	70	44.758	-1.736	97.832	1.00	40.00
ATOM	565	N	THR	71	43.470	-3.517	97.280	1.00	20.00
ATOM	566	CA	THR	71	43.052	-3.866	98.612	1.00	20.00
ATOM	567	CB	THR	71	44.152	-4.465	99.444	1.00	20.00
ATOM	568	OG1	THR	71	45.227	-3.551	99.595	1.00	20.00
ATOM	569	CG2	THR	71	44.640	-5.747	98.748	1.00	20.00
ATOM	570	C	THR	71	42.444	-2.701	99.332	1.00	20.00
ATOM	571	O	THR	71	42.100	-2.811	100.509	1.00	20.00
ATOM	572	N	VAL	72	42.258	-1.558	98.649	1.00	20.00
ATOM	573	CA	VAL	72	41.644	-0.442	99.303	1.00	20.00
ATOM	574	CB	VAL	72	42.202	0.880	98.865	1.00	20.00
ATOM	575	CG1	VAL	72	41.433	2.002	99.581	1.00	20.00
ATOM	576	CG2	VAL	72	43.713	0.883	99.152	1.00	20.00
ATOM	577	C	VAL	72	40.201	-0.486	98.919	1.00	20.00
ATOM	578	O	VAL	72	39.857	-0.358	97.746	1.00	20.00
ATOM	579	N	GLU	73	39.327	-0.717	99.915	1.00	20.00
ATOM	580	CA	GLU	73	37.915	-0.843	99.701	1.00	20.00
ATOM	581	CB	GLU	73	37.194	-1.339	100.963	1.00	20.00
ATOM	582	CG	GLU	73	37.640	-2.744	101.372	1.00	20.00
ATOM	583	CD	GLU	73	36.928	-3.110	102.666	1.00	20.00
ATOM	584	OE1	GLU	73	36.063	-2.311	103.113	1.00	20.00
ATOM	585	OE2	GLU	73	37.239	-4.194	103.228	1.00	20.00
ATOM	586	C	GLU	73	37.316	0.470	99.306	1.00	20.00
ATOM	587	O	GLU	73	36.516	0.533	98.375	1.00	20.00
ATOM	588	N	ARG	74	37.683	1.567	99.997	1.00	20.00
ATOM	589	CA	ARG	74	37.070	2.827	99.686	1.00	20.00
ATOM	590	CB	ARG	74	35.789	3.070	100.496	1.00	20.00
ATOM	591	CG	ARG	74	36.045	3.117	102.003	1.00	20.00
ATOM	592	CD	ARG	74	34.812	2.787	102.845	1.00	20.00
ATOM	593	NE	ARG	74	34.771	1.303	102.979	1.00	20.00
ATOM	594	CZ	ARG	74	33.882	0.711	103.828	1.00	20.00
ATOM	595	NH1	ARG	74	32.999	1.476	104.533	1.00	20.00
ATOM	596	NH2	ARG	74	33.879	-0.646	103.970	1.00	20.00
ATOM	597	C	ARG	74	38.041	3.891	100.087	1.00	20.00
ATOM	598	O	ARG	74	39.121	3.600	100.564	1.00	20.00
ATOM	599	N	ILE	75	37.703	5.166	99.786	1.00	20.00
ATOM	600	CA	ILE	75	38.585	6.208	100.225	1.00	20.00
ATOM	601	CB	ILE	75	39.043	7.136	99.134	1.00	20.00
ATOM	602	CG2	ILE	75	37.817	7.778	98.460	1.00	20.00
ATOM	603	CG1	ILE	75	40.071	8.131	99.702	1.00	20.00
ATOM	604	CD1	ILE	75	40.836	8.911	98.634	1.00	20.00
ATOM	605	C	ILE	75	37.853	7.001	101.261	1.00	20.00
ATOM	606	O	ILE	75	37.671	8.211	101.160	1.00	20.00
ATOM	607	N	PRO	76	37.535	6.301	102.310	1.00	20.00
ATOM	608	CA	PRO	76	36.674	6.739	103.368	1.00	20.00
ATOM	609	CD	PRO	76	38.383	5.207	102.753	1.00	20.00
ATOM	610	CB	PRO	76	36.562	5.541	104.303	1.00	20.00
ATOM	611	CG	PRO	76	37.957	4.907	104.199	1.00	20.00
ATOM	612	C	PRO	76	37.213	7.895	104.164	1.00	20.00
ATOM	613	O	PRO	76	36.616	8.128	105.194	1.00	20.00
ATOM	614	N	LEU	77	38.343	8.534	103.731	1.00	20.00
ATOM	615	CA	LEU	77	38.864	9.725	104.379	1.00	20.00
ATOM	616	CB	LEU	77	39.775	10.571	103.467	1.00	20.00

Figure 6 (continued)

ATOM	617	CG	LEU	77	41.107	9.897	103.114	1.00	20.00
ATOM	618	CD1	LEU	77	41.968	10.791	102.207	1.00	20.00
ATOM	619	CD2	LEU	77	41.848	9.468	104.385	1.00	20.00
ATOM	620	C	LEU	77	37.678	10.573	104.701	1.00	20.00
ATOM	621	O	LEU	77	37.135	11.270	103.847	1.00	20.00
ATOM	622	N	GLU	78	37.263	10.523	105.980	1.00	20.00
ATOM	623	CA	GLU	78	36.010	11.071	106.401	1.00	20.00
ATOM	624	CB	GLU	78	35.733	10.830	107.895	1.00	20.00
ATOM	625	CG	GLU	78	35.522	9.357	108.252	1.00	20.00
ATOM	626	CD	GLU	78	35.263	9.275	109.750	1.00	20.00
ATOM	627	OE1	GLU	78	35.743	10.178	110.485	1.00	20.00
ATOM	628	OE2	GLU	78	34.577	8.308	110.180	1.00	20.00
ATOM	629	C	GLU	78	36.939	12.545	106.181	1.00	20.00
ATOM	630	O	GLU	78	34.935	13.043	105.683	1.00	20.00
ATOM	631	N	ASN	79	37.005	13.274	106.548	1.00	20.00
ATOM	632	CA	ASN	79	37.018	14.711	106.554	1.00	20.00
ATOM	633	CB	ASN	79	38.156	15.300	107.401	1.00	20.00
ATOM	634	CG	ASN	79	37.761	15.120	108.858	1.00	20.00
ATOM	635	OD1	ASN	79	37.588	14.003	109.343	1.00	20.00
ATOM	636	ND2	ASN	79	37.601	16.260	109.581	1.00	20.00
ATOM	637	C	ASN	79	37.063	15.387	105.216	1.00	20.00
ATOM	638	O	ASN	79	36.550	16.500	105.119	1.00	20.00
ATOM	639	N	LEU	80	37.681	14.769	104.183	1.00	20.00
ATOM	640	CA	LEU	80	37.952	15.381	102.896	1.00	20.00
ATOM	641	CB	LEU	80	38.244	14.333	101.805	1.00	20.00
ATOM	642	CG	LEU	80	38.538	14.936	100.420	1.00	20.00
ATOM	643	CD1	LEU	80	39.837	15.762	100.442	1.00	20.00
ATOM	644	CD2	LEU	80	38.542	13.854	99.330	1.00	20.00
ATOM	645	C	LEU	80	36.792	16.221	102.430	1.00	20.00
ATOM	646	O	LEU	80	35.806	15.703	101.910	1.00	20.00
ATOM	647	N	GLN	81	36.880	17.544	102.714	1.00	20.00
ATOM	648	CA	GLN	81	35.908	18.567	102.408	1.00	20.00
ATOM	649	CB	GLN	81	36.105	19.797	103.309	1.00	20.00
ATOM	650	CG	GLN	81	36.195	19.478	104.804	1.00	20.00
ATOM	651	CD	GLN	81	34.852	18.957	105.288	1.00	20.00
ATOM	652	OE1	GLN	81	34.703	18.599	106.455	1.00	20.00
ATOM	653	NE2	GLN	81	33.847	18.914	104.373	1.00	20.00
ATOM	654	C	GLN	81	35.951	19.113	101.000	1.00	20.00
ATOM	655	O	GLN	81	34.917	19.216	100.342	1.00	20.00
ATOM	656	N	ILE	82	37.144	19.517	100.500	1.00	20.00
ATOM	657	CA	ILE	82	37.179	20.183	99.221	1.00	20.00
ATOM	658	CB	ILE	82	37.036	21.674	99.331	1.00	20.00
ATOM	659	CG2	ILE	82	38.255	22.209	100.098	1.00	20.00
ATOM	660	CG1	ILE	82	36.846	22.303	97.941	1.00	20.00
ATOM	661	CD1	ILE	82	36.418	23.770	97.983	1.00	20.00
ATOM	662	C	ILE	82	38.486	19.931	98.535	1.00	20.00
ATOM	663	O	ILE	82	39.512	19.721	99.182	1.00	20.00
ATOM	664	N	ILE	83	38.463	19.933	97.183	1.00	20.00
ATOM	665	CA	ILE	83	39.639	19.776	96.369	1.00	20.00
ATOM	666	CB	ILE	83	39.580	18.550	95.503	1.00	20.00
ATOM	667	CG2	ILE	83	40.815	18.541	94.587	1.00	20.00
ATOM	668	CG1	ILE	83	39.446	17.289	96.373	1.00	20.00
ATOM	669	CD1	ILE	83	39.047	16.047	95.580	1.00	20.00
ATOM	670	C	ILE	83	39.638	20.964	95.451	1.00	20.00
ATOM	671	O	ILE	83	38.949	20.969	94.436	1.00	20.00
ATOM	672	N	ARG	84	40.475	21.974	95.739	1.00	20.00
ATOM	673	CA	ARG	84	40.438	23.237	95.051	1.00	20.00
ATOM	674	CB	ARG	84	41.379	24.292	95.663	1.00	20.00
ATOM	675	CG	ARG	84	41.086	24.532	97.144	1.00	20.00
ATOM	676	CD	ARG	84	41.913	25.688	97.804	1.00	20.00
ATOM	677	NE	ARG	84	41.337	26.957	97.179	1.00	20.00
ATOM	678	CZ	ARG	84	40.267	27.637	97.693	1.00	20.00
ATOM	679	NH1	ARG	84	39.610	27.185	98.804	1.00	20.00
ATOM	680	NH2	ARG	84	39.851	28.788	97.090	1.00	20.00
ATOM	681	C	ARG	84	40.670	23.120	93.575	1.00	20.00
ATOM	682	O	ARG	84	40.120	23.908	92.809	1.00	20.00
ATOM	683	N	GLY	85	41.524	22.192	93.117	1.00	20.00
ATOM	684	CA	GLY	85	41.729	22.083	91.698	1.00	20.00
ATOM	685	C	GLY	85	42.603	23.201	91.212	1.00	20.00
ATOM	686	O	GLY	85	42.529	23.552	90.048	1.00	20.00
ATOM	687	N	ASN	86	43.476	23.734	92.087	1.00	20.00
ATOM	688	CA	ASN	86	44.351	24.804	91.696	1.00	20.00
ATOM	689	CB	ASN	86	45.378	25.141	92.790	1.00	20.00
ATOM	690	CG	ASN	86	46.262	26.275	92.294	1.00	20.00
ATOM	691	OD1	ASN	86	46.903	26.998	91.366	1.00	20.00
ATOM	692	ND2	ASN	86	47.457	26.428	92.924	1.00	20.00
ATOM	693	C	ASN	86	45.130	24.312	90.520	1.00	20.00

Figure 6 (continued)

ATOM	694	O	ASN	86	45.319	25.026	89.536	1.00	20.00
ATOM	695	N	MET	87	45.617	23.064	90.600	1.00	20.00
ATOM	696	CA	MET	87	46.314	22.475	89.508	1.00	20.00
ATOM	697	CB	MET	87	47.798	22.195	89.796	1.00	20.00
ATOM	698	CG	MET	87	48.622	23.467	89.999	1.00	20.00
ATOM	699	SD	MET	87	50.375	23.181	90.389	1.00	20.00
ATOM	700	CE	MET	87	50.052	22.614	92.084	1.00	20.00
ATOM	701	C	MET	87	45.644	21.165	89.296	1.00	20.00
ATOM	702	O	MET	87	45.346	20.450	90.240	1.00	20.00
ATOM	703	N	TYR	88	45.396	20.807	88.016	1.00	20.00
ATOM	704	CA	TYR	88	44.662	19.593	87.805	1.00	20.00
ATOM	705	CB	TYR	88	43.276	19.806	87.169	1.00	20.00
ATOM	706	CG	TYR	88	43.437	20.643	85.946	1.00	20.00
ATOM	707	CD1	TYR	88	43.781	20.077	84.742	1.00	20.00
ATOM	708	CD2	TYR	88	43.258	22.005	86.011	1.00	20.00
ATOM	709	CE1	TYR	88	43.926	20.850	83.615	1.00	20.00
ATOM	710	CE2	TYR	88	43.403	22.787	84.888	1.00	20.00
ATOM	711	CZ	TYR	88	43.737	22.207	83.687	1.00	20.00
ATOM	712	OH	TYR	88	43.885	23.004	82.532	1.00	20.00
ATOM	713	C	TYR	88	45.425	18.639	86.952	1.00	20.00
ATOM	714	O	TYR	88	46.402	18.994	86.293	1.00	20.00
ATOM	715	N	TYR	89	44.984	17.364	86.998	1.00	20.00
ATOM	716	CA	TYR	89	45.547	16.309	86.214	1.00	20.00
ATOM	717	CB	TYR	89	44.896	14.946	86.509	1.00	20.00
ATOM	718	CG	TYR	89	45.687	13.873	85.844	1.00	20.00
ATOM	719	CD1	TYR	89	46.827	13.387	86.441	1.00	20.00
ATOM	720	CD2	TYR	89	45.290	13.343	84.639	1.00	20.00
ATOM	721	CE1	TYR	89	47.566	12.394	85.844	1.00	20.00
ATOM	722	CE2	TYR	89	46.025	12.348	84.036	1.00	20.00
ATOM	723	CZ	TYR	89	47.165	11.873	84.639	1.00	20.00
ATOM	724	OH	TYR	89	47.920	10.853	84.022	1.00	20.00
ATOM	725	C	TYR	89	45.244	16.696	84.806	1.00	20.00
ATOM	726	O	TYR	89	44.261	17.387	84.555	1.00	20.00
ATOM	727	N	GLU	90	46.061	16.198	83.856	1.00	20.00
ATOM	728	CA	GLU	90	46.054	16.661	82.499	1.00	20.00
ATOM	729	CB	GLU	90	46.848	15.747	81.554	1.00	20.00
ATOM	730	CG	GLU	90	47.131	16.399	80.202	1.00	20.00
ATOM	731	CD	GLU	90	48.086	17.557	80.456	1.00	20.00
ATOM	732	OE1	GLU	90	48.382	17.828	81.651	1.00	20.00
ATOM	733	OE2	GLU	90	48.535	18.189	79.467	1.00	20.00
ATOM	734	C	GLU	90	44.696	16.847	81.911	1.00	20.00
ATOM	735	O	GLU	90	44.369	17.952	81.480	1.00	20.00
ATOM	736	N	ASN	91	43.842	15.807	81.891	1.00	20.00
ATOM	737	CA	ASN	91	42.583	15.998	81.226	1.00	20.00
ATOM	738	CB	ASN	91	41.895	14.683	80.852	1.00	20.00
ATOM	739	CG	ASN	91	40.821	15.007	79.790	1.00	20.00
ATOM	740	OD1	ASN	91	40.502	16.168	79.540	1.00	20.00
ATOM	741	ND2	ASN	91	40.244	13.944	79.168	1.00	20.00
ATOM	742	C	ASN	91	41.654	16.782	82.103	1.00	20.00
ATOM	743	O	ASN	91	40.436	16.618	82.049	1.00	20.00
ATOM	744	N	SER	92	42.217	17.685	82.928	1.00	20.00
ATOM	745	CA	SER	92	41.458	18.550	83.771	1.00	20.00
ATOM	746	CB	SER	92	40.411	19.377	83.005	1.00	20.00
ATOM	747	OG	SER	92	41.053	20.266	82.105	1.00	20.00
ATOM	748	C	SER	92	40.740	17.743	84.795	1.00	20.00
ATOM	749	O	SER	92	39.548	17.946	85.011	1.00	20.00
ATOM	750	N	TYR	93	41.445	16.816	85.473	1.00	20.00
ATOM	751	CA	TYR	93	40.754	16.048	86.465	1.00	20.00
ATOM	752	CB	TYR	93	40.931	14.526	86.323	1.00	20.00
ATOM	753	CG	TYR	93	40.207	14.111	85.087	1.00	20.00
ATOM	754	CD1	TYR	93	38.833	14.096	85.062	1.00	20.00
ATOM	755	CD2	TYR	93	40.892	13.724	83.959	1.00	20.00
ATOM	756	CE1	TYR	93	38.150	13.713	83.933	1.00	20.00
ATOM	757	CE2	TYR	93	40.211	13.339	82.828	1.00	20.00
ATOM	758	CZ	TYR	93	38.839	13.335	82.809	1.00	20.00
ATOM	759	OH	TYR	93	38.146	12.941	81.645	1.00	20.00
ATOM	760	C	TYR	93	41.222	16.439	87.832	1.00	20.00
ATOM	761	O	TYR	93	42.414	16.457	88.129	1.00	20.00
ATOM	762	N	ALA	94	40.261	16.856	88.676	1.00	20.00
ATOM	763	CA	ALA	94	40.483	17.180	90.055	1.00	20.00
ATOM	764	CB	ALA	94	39.342	18.017	90.662	1.00	20.00
ATOM	765	C	ALA	94	40.581	15.919	90.851	1.00	20.00
ATOM	766	O	ALA	94	41.329	15.847	91.824	1.00	20.00
ATOM	767	N	LEU	95	39.774	14.906	90.473	1.00	20.00
ATOM	768	CA	LEU	95	39.719	13.653	91.173	1.00	20.00
ATOM	769	CB	LEU	95	38.354	13.459	91.861	1.00	20.00
ATOM	770	CG	LEU	95	38.094	12.070	92.472	1.00	20.00

Figure 6 (continued)

ATOM	771	CD1	LEU	95	39.069	11.743	93.609	1.00	20.00
ATOM	772	CD2	LEU	95	36.623	11.933	92.905	1.00	20.00
ATOM	773	C	LEU	95	39.876	12.559	90.167	1.00	20.00
ATOM	774	O	LEU	95	38.961	12.291	89.383	1.00	20.00
ATOM	775	N	ALA	96	41.031	11.882	90.164	1.00	20.00
ATOM	776	CA	ALA	96	41.200	10.812	89.228	1.00	20.00
ATOM	777	CB	ALA	96	42.470	10.941	88.368	1.00	20.00
ATOM	778	C	ALA	96	41.329	9.551	90.013	1.00	20.00
ATOM	779	O	ALA	96	42.199	9.438	90.874	1.00	20.00
ATOM	780	N	VAL	97	40.424	8.584	89.761	1.00	20.00
ATOM	781	CA	VAL	97	40.531	7.299	90.381	1.00	20.00
ATOM	782	CB	VAL	97	39.363	6.955	91.271	1.00	20.00
ATOM	783	CG1	VAL	97	39.424	7.874	92.503	1.00	20.00
ATOM	784	CG2	VAL	97	38.046	7.115	90.490	1.00	20.00
ATOM	785	C	VAL	97	40.626	6.319	89.253	1.00	20.00
ATOM	786	O	VAL	97	39.652	6.044	88.555	1.00	20.00
ATOM	787	N	LEU	98	41.820	5.743	89.036	1.00	20.00
ATOM	788	CA	LEU	98	41.928	4.905	87.883	1.00	20.00
ATOM	789	CB	LEU	98	42.951	5.434	86.864	1.00	20.00
ATOM	790	CG	LEU	98	42.656	6.870	86.390	1.00	20.00
ATOM	791	CD1	LEU	98	43.675	7.332	85.335	1.00	20.00
ATOM	792	CD2	LEU	98	41.199	7.031	85.934	1.00	20.00
ATOM	793	C	LEU	98	42.392	3.552	88.296	1.00	20.00
ATOM	794	O	LEU	98	43.270	3.424	89.148	1.00	20.00
ATOM	795	N	SER	99	41.794	2.516	87.669	1.00	20.00
ATOM	796	CA	SER	99	42.134	1.136	87.873	1.00	20.00
ATOM	797	CB	SER	99	43.417	0.713	87.138	1.00	20.00
ATOM	798	OG	SER	99	43.242	0.839	85.735	1.00	20.00
ATOM	799	C	SER	99	42.335	0.871	89.327	1.00	20.00
ATOM	800	O	SER	99	43.443	0.555	89.755	1.00	20.00
ATOM	801	N	ASN	100	41.270	1.019	90.134	1.00	40.00
ATOM	802	CA	ASN	100	41.424	0.743	91.529	1.00	40.00
ATOM	803	CB	ASN	100	40.691	1.735	92.448	1.00	40.00
ATOM	804	CG	ASN	100	41.518	3.011	92.524	1.00	40.00
ATOM	805	OD1	ASN	100	41.325	3.950	91.753	1.00	40.00
ATOM	806	ND2	ASN	100	42.469	3.050	93.495	1.00	40.00
ATOM	807	C	ASN	100	40.850	-0.608	91.768	1.00	40.00
ATOM	808	O	ASN	100	39.636	-0.793	91.798	1.00	40.00
ATOM	809	N	TYR	101	41.744	-1.602	91.912	1.00	40.00
ATOM	810	CA	TYR	101	41.306	-2.957	92.024	1.00	40.00
ATOM	811	CB	TYR	101	41.928	-3.882	90.963	1.00	40.00
ATOM	812	CG	TYR	101	41.573	-3.386	89.604	1.00	40.00
ATOM	813	CD1	TYR	101	42.196	-2.271	89.092	1.00	40.00
ATOM	814	CD2	TYR	101	40.643	-4.043	88.832	1.00	40.00
ATOM	815	CE1	TYR	101	41.885	-1.805	87.837	1.00	40.00
ATOM	816	CE2	TYR	101	40.330	-3.583	87.574	1.00	40.00
ATOM	817	CZ	TYR	101	40.949	-2.462	87.076	1.00	40.00
ATOM	818	OH	TYR	101	40.628	-1.989	85.786	1.00	40.00
ATOM	819	C	TYR	101	41.795	-3.497	93.322	1.00	40.00
ATOM	820	O	TYR	101	42.252	-2.770	94.202	1.00	40.00
ATOM	821	N	ASP	102	41.681	-4.830	93.440	1.00	60.00
ATOM	822	CA	ASP	102	42.123	-5.534	94.562	1.00	60.00
ATOM	823	CB	ASP	102	40.964	-6.200	95.376	1.00	60.00
ATOM	824	CG	ASP	102	41.496	-6.734	96.697	1.00	60.00
ATOM	825	OD1	ASP	102	42.710	-6.541	96.970	1.00	60.00
ATOM	826	OD2	ASP	102	40.693	-7.345	97.452	1.00	60.00
ATOM	827	C	ASP	102	42.861	-6.724	93.929	1.00	60.00
ATOM	828	O	ASP	102	43.134	-6.686	92.729	1.00	60.00
ATOM	829	N	ALA	103	43.225	-7.756	94.709	1.00	60.00
ATOM	830	CA	ALA	103	43.893	-8.865	94.104	1.00	60.00
ATOM	831	CB	ALA	103	44.202	-9.996	95.099	1.00	60.00
ATOM	832	C	ALA	103	42.923	-9.393	93.102	1.00	60.00
ATOM	833	O	ALA	103	43.286	-9.729	91.976	1.00	60.00
ATOM	834	N	ASN	104	41.641	-9.448	93.502	1.00	60.00
ATOM	835	CA	ASN	104	40.604	-9.896	92.625	1.00	60.00
ATOM	836	CB	ASN	104	39.414	-10.537	93.359	1.00	60.00
ATOM	837	CG	ASN	104	39.899	-11.855	93.949	1.00	60.00
ATOM	838	OD1	ASN	104	40.883	-12.429	93.485	1.00	60.00
ATOM	839	ND2	ASN	104	39.189	-12.352	94.997	1.00	60.00
ATOM	840	C	ASN	104	40.102	-8.722	91.880	1.00	60.00
ATOM	841	O	ASN	104	40.658	-7.610	91.981	1.00	60.00
ATOM	842	N	LYS	105	39.031	-8.901	91.090	1.00	60.00
ATOM	843	CA	LYS	105	38.458	-7.851	90.301	1.00	60.00
ATOM	844	CB	LYS	105	37.253	-8.323	89.471	1.00	60.00
ATOM	845	CG	LYS	105	37.606	-9.373	88.415	1.00	60.00
ATOM	846	CD	LYS	105	38.031	-10.717	89.010	1.00	60.00
ATOM	847	CE	LYS	105	38.386	-11.771	87.958	1.00	60.00

Figure 6 (continued)

ATOM	848	NZ	LYS	105	37.175	-12.149	97.195	1.00	60.00
ATOM	849	C	LYS	105	37.972	-6.794	91.237	1.00	60.00
ATOM	850	O	LYS	105	38.074	-5.601	90.953	1.00	60.00
ATOM	851	N	THR	106	37.438	-7.217	92.397	1.00	60.00
ATOM	852	CA	THR	106	36.902	-6.318	93.378	1.00	60.00
ATOM	853	CB	THR	106	36.226	-7.076	94.496	1.00	60.00
ATOM	854	OG1	THR	106	35.283	-7.980	93.939	1.00	60.00
ATOM	855	CG2	THR	106	35.461	-6.112	95.423	1.00	60.00
ATOM	856	C	THR	106	38.064	-5.520	93.916	1.00	60.00
ATOM	857	O	THR	106	39.174	-5.602	93.387	1.00	60.00
ATOM	858	N	GLY	107	37.841	-4.704	94.959	1.00	60.00
ATOM	859	CA	GLY	107	38.690	-3.902	95.815	1.00	60.00
ATOM	860	C	GLY	107	38.297	-2.600	95.946	1.00	60.00
ATOM	861	O	GLY	107	38.185	-2.344	97.144	1.00	60.00
ATOM	862	N	LEU	108	37.892	-1.730	95.002	1.00	20.00
ATOM	863	CA	LEU	108	37.286	-0.514	95.481	1.00	20.00
ATOM	864	CB	LEU	108	37.761	0.736	94.725	1.00	20.00
ATOM	865	CG	LEU	108	37.132	2.051	95.221	1.00	20.00
ATOM	866	CD1	LEU	108	37.587	2.382	96.651	1.00	20.00
ATOM	867	CD2	LEU	108	37.392	3.199	94.236	1.00	20.00
ATOM	868	C	LEU	108	35.808	-0.622	95.296	1.00	20.00
ATOM	869	O	LEU	108	35.310	-0.562	94.175	1.00	20.00
ATOM	870	N	LYS	109	35.080	-0.834	96.407	1.00	20.00
ATOM	871	CA	LYS	109	33.652	-0.972	96.422	1.00	20.00
ATOM	872	CB	LYS	109	33.177	-1.888	97.746	1.00	20.00
ATOM	873	CG	LYS	109	33.781	-2.980	97.942	1.00	20.00
ATOM	874	CD	LYS	109	33.705	-3.514	99.371	1.00	20.00
ATOM	875	CE	LYS	109	34.435	-4.847	99.554	1.00	20.00
ATOM	876	NZ	LYS	109	35.900	-4.636	99.510	1.00	20.00
ATOM	877	C	LYS	109	32.969	0.346	96.216	1.00	20.00
ATOM	878	O	LYS	109	31.967	0.426	95.508	1.00	20.00
ATOM	879	N	GLU	110	33.479	1.428	96.838	1.00	20.00
ATOM	880	CA	GLU	110	32.917	2.691	96.712	1.00	20.00
ATOM	881	CB	GLU	110	31.570	2.777	97.609	1.00	20.00
ATOM	882	CG	GLU	110	31.790	2.191	99.006	1.00	20.00
ATOM	883	CD	GLU	110	30.514	2.388	99.813	1.00	20.00
ATOM	884	OE1	GLU	110	29.628	3.150	99.342	1.00	20.00
ATOM	885	OE2	GLU	110	30.409	1.781	100.912	1.00	20.00
ATOM	886	C	GLU	110	33.783	3.774	97.071	1.00	20.00
ATOM	887	O	GLU	110	34.925	3.502	97.431	1.00	20.00
ATOM	888	N	LEU	111	33.352	5.041	96.877	1.00	20.00
ATOM	889	CA	LEU	111	34.081	6.238	97.206	1.00	20.00
ATOM	890	CB	LEU	111	33.635	7.432	96.373	1.00	20.00
ATOM	891	CG	LEU	111	33.957	7.309	94.874	1.00	20.00
ATOM	892	CD1	LEU	111	33.534	8.562	94.088	1.00	20.00
ATOM	893	CD2	LEU	111	35.433	6.930	94.658	1.00	20.00
ATOM	894	C	LEU	111	34.016	6.650	98.671	1.00	20.00
ATOM	895	O	LEU	111	35.004	7.215	99.134	1.00	20.00
ATOM	896	N	PRO	112	32.985	6.311	99.441	1.00	20.00
ATOM	897	CA	PRO	112	32.657	7.027	100.668	1.00	20.00
ATOM	898	CD	PRO	112	32.920	4.888	99.729	1.00	20.00
ATOM	899	CB	PRO	112	32.502	6.009	101.799	1.00	20.00
ATOM	900	CG	PRO	112	33.114	4.728	101.239	1.00	20.00
ATOM	901	C	PRO	112	33.422	8.238	101.103	1.00	20.00
ATOM	902	O	PRO	112	33.888	8.320	102.236	1.00	20.00
ATOM	903	N	MET	113	33.441	9.227	100.204	1.00	20.00
ATOM	904	CA	MET	113	33.992	10.547	100.278	1.00	20.00
ATOM	905	CB	MET	113	34.370	11.152	98.914	1.00	20.00
ATOM	906	CG	MET	113	35.593	10.495	98.271	1.00	20.00
ATOM	907	SD	MET	113	36.060	11.195	96.659	1.00	20.00
ATOM	908	CE	MET	113	37.578	10.213	96.488	1.00	20.00
ATOM	909	C	MET	113	32.967	11.442	100.897	1.00	20.00
ATOM	910	O	MET	113	32.986	12.634	100.634	1.00	20.00
ATOM	911	N	ARG	114	32.006	10.898	101.670	1.00	20.00
ATOM	912	CA	ARG	114	30.791	11.572	102.067	1.00	20.00
ATOM	913	CH	ARG	114	30.082	10.907	103.264	1.00	20.00
ATOM	914	CG	ARG	114	30.878	10.927	104.569	1.00	20.00
ATOM	915	CD	ARG	114	30.118	10.306	105.744	1.00	20.00
ATOM	916	NE	ARG	114	28.888	11.122	105.958	1.00	20.00
ATOM	917	CZ	ARG	114	28.896	12.171	106.832	1.00	20.00
ATOM	918	NH1	ARG	114	30.027	12.467	107.538	1.00	20.00
ATOM	919	NH2	ARG	114	27.770	12.923	107.000	1.00	20.00
ATOM	920	C	ARG	114	30.943	13.031	102.415	1.00	20.00
ATOM	921	O	ARG	114	30.010	13.792	102.177	1.00	20.00
ATOM	922	N	ASN	115	32.050	13.477	103.024	1.00	20.00
ATOM	923	CA	ASN	115	32.208	14.868	103.374	1.00	20.00
ATOM	924	CB	ASN	115	33.263	15.108	104.462	1.00	20.00

Figure 6 (continued)

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ATOM    925  CG  ASN   115      32.622  14.667 105.771  1.00 20.00
ATOM    926  OD1 ASN   115      31.474  14.228 105.797  1.00 20.00
ATOM    927  ND2 ASN   115      33.369  14.812 106.896  1.00 20.00
ATOM    928  C   ASN   115      32.512  15.762 102.193  1.00 20.00
ATOM    929  O   ASN   115      32.475  16.985 102.328  1.00 20.00
ATOM    930  N   LEU   116      32.874  15.197 101.027  1.00 20.00
ATOM    931  CA  LEU   116      33.324  15.949  99.887  1.00 20.00
ATOM    932  CB  LEU   116      33.891  15.048  98.774  1.00 20.00
ATOM    933  CG  LEU   116      34.406  15.807  97.541  1.00 20.00
ATOM    934  CD1 LEU   116      35.587  16.720  97.907  1.00 20.00
ATOM    935  CD2 LEU   116      34.751  14.836  96.401  1.00 20.00
ATOM    936  C   LEU   116      32.208  16.778  99.318  1.00 20.00
ATOM    937  O   LEU   116      31.331  16.276  98.617  1.00 20.00
ATOM    938  N   GLN   117      32.201  18.074  99.699  1.00 20.00
ATOM    939  CA  GLN   117      31.258  19.080  99.298  1.00 20.00
ATOM    940  CB  GLN   117      31.161  20.221 100.327  1.00 20.00
ATOM    941  CG  GLN   117      30.430  19.854 101.620  1.00 20.00
ATOM    942  CD  GLN   117      28.941  20.045 101.368  1.00 20.00
ATOM    943  OE1 GLN   117      28.107  19.778 102.231  1.00 20.00
ATOM    944  NE2 GLN   117      28.594  20.532 100.146  1.00 20.00
ATOM    945  C   GLN   117      31.549  19.738  97.980  1.00 20.00
ATOM    946  O   GLN   117      30.616  20.069  97.255  1.00 20.00
ATOM    947  N   GLU   118      32.825  20.024  97.640  1.00 20.00
ATOM    948  CA  GLU   118      32.991  20.755  96.414  1.00 20.00
ATOM    949  CB  GLU   118      32.814  22.274  96.583  1.00 20.00
ATOM    950  CG  GLU   118      31.386  22.711  96.912  1.00 20.00
ATOM    951  CD  GLU   118      31.397  24.228  97.045  1.00 20.00
ATOM    952  OE1 GLU   118      32.502  24.820  96.919  1.00 20.00
ATOM    953  OE2 GLU   118      30.306  24.815  97.200  1.00 20.00
ATOM    954  C   GLU   118      34.359  20.564  95.847  1.00 20.00
ATOM    955  O   GLU   118      35.346  20.459  96.573  1.00 20.00
ATOM    956  N   ILE   119      34.430  20.506  94.501  1.00 20.00
ATOM    957  CA  ILE   119      35.680  20.480  93.804  1.00 20.00
ATOM    958  CB  ILE   119      35.809  19.351  92.818  1.00 20.00
ATOM    959  CG2 ILE   119      37.074  19.581  91.976  1.00 20.00
ATOM    960  CG1 ILE   119      35.802  18.001  93.555  1.00 20.00
ATOM    961  CD1 ILE   119      35.706  16.791  92.626  1.00 20.00
ATOM    962  C   ILE   119      35.709  21.770  93.052  1.00 20.00
ATOM    963  O   ILE   119      35.224  21.861  91.926  1.00 20.00
ATOM    964  N   LEU   120      36.396  22.773  93.625  1.00 20.00
ATOM    965  CA  LEU   120      36.373  24.132  93.162  1.00 20.00
ATOM    966  CB  LEU   120      37.433  25.005  93.855  1.00 20.00
ATOM    967  CG  LEU   120      37.439  26.469  93.379  1.00 20.00
ATOM    968  CD1 LEU   120      36.125  27.179  93.746  1.00 20.00
ATOM    969  CD2 LEU   120      38.685  27.215  93.877  1.00 20.00
ATOM    970  C   LEU   120      36.652  24.185  91.695  1.00 20.00
ATOM    971  O   LEU   120      36.082  25.024  90.999  1.00 20.00
ATOM    972  N   HIS   121      37.550  23.334  91.164  1.00 20.00
ATOM    973  CA  HIS   121      37.743  23.442  89.747  1.00 20.00
ATOM    974  ND1 HIS   121      37.979  25.853  87.395  1.00 20.00
ATOM    975  NE2 HIS   121      39.013  24.938  85.652  1.00 20.00
ATOM    976  CE1 HIS   121      38.173  25.875  86.053  1.00 20.00
ATOM    977  CD2 HIS   121      39.379  24.279  86.812  1.00 20.00
ATOM    978  CG  HIS   121      38.754  24.827  87.891  1.00 20.00
ATOM    979  CB  HIS   121      38.820  24.461  89.344  1.00 20.00
ATOM    980  C   HIS   121      38.157  22.111  89.206  1.00 20.00
ATOM    981  O   HIS   121      38.717  21.281  89.920  1.00 20.00
ATOM    982  N   GLY   122      37.876  21.878  87.907  1.00 20.00
ATOM    983  CA  GLY   122      38.266  20.659  87.263  1.00 20.00
ATOM    984  C   GLY   122      37.146  19.672  87.386  1.00 20.00
ATOM    985  O   GLY   122      36.209  19.872  88.158  1.00 20.00
ATOM    986  N   ALA   123      37.239  18.576  86.599  1.00 20.00
ATOM    987  CA  ALA   123      36.262  17.523  86.553  1.00 20.00
ATOM    988  CB  ALA   123      35.947  17.049  85.122  1.00 20.00
ATOM    989  C   ALA   123      36.781  16.328  87.296  1.00 20.00
ATOM    990  O   ALA   123      37.767  16.415  88.023  1.00 20.00
ATOM    991  N   VAL   124      36.091  15.174  87.150  1.00 20.00
ATOM    992  CA  VAL   124      36.495  13.953  87.799  1.00 20.00
ATOM    993  CB  VAL   124      35.513  13.479  88.830  1.00 20.00
ATOM    994  CG1 VAL   124      36.036  12.172  89.447  1.00 20.00
ATOM    995  CG2 VAL   124      35.297  14.606  89.854  1.00 20.00
ATOM    996  C   VAL   124      36.598  12.871  86.761  1.00 20.00
ATOM    997  O   VAL   124      35.978  12.958  85.704  1.00 20.00
ATOM    998  N   ARG   125      37.431  11.834  87.011  1.00 20.00
ATOM    999  CA  ARG   125      37.499  10.738  86.083  1.00 20.00
ATOM   1000  CB  ARG   125      38.785  10.700  85.246  1.00 20.00
ATOM   1001  CG  ARG   125      38.867   9.479  84.329  1.00 20.00
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Figure 6 (continued)

ATOM	1002	CD	ARG	125	39.979	9.589	83.289	1.00	20.00
ATOM	1003	NE	ARG	125	41.137	10.238	83.961	1.00	20.00
ATOM	1004	CZ	ARG	125	42.061	10.906	83.213	1.00	20.00
ATOM	1005	NH1	ARG	125	41.961	10.909	81.852	1.00	20.00
ATOM	1006	NH2	ARG	125	43.075	11.584	83.824	1.00	20.00
ATOM	1007	C	ARG	125	37.433	9.452	86.847	1.00	20.00
ATOM	1008	O	ARG	125	38.360	9.097	87.572	1.00	20.00
ATOM	1009	N	PHE	126	36.329	8.698	86.690	1.00	20.00
ATOM	1010	CA	PHE	126	36.228	7.446	87.385	1.00	20.00
ATOM	1011	CB	PHE	126	34.851	7.195	88.031	1.00	20.00
ATOM	1012	CG	PHE	126	34.507	8.261	89.012	1.00	20.00
ATOM	1013	CD1	PHE	126	34.990	8.228	90.294	1.00	20.00
ATOM	1014	CD2	PHE	126	33.671	9.287	88.639	1.00	20.00
ATOM	1015	CE1	PHE	126	34.653	9.216	91.194	1.00	20.00
ATOM	1016	CE2	PHE	126	33.330	10.277	89.530	1.00	20.00
ATOM	1017	CZ	PHE	126	33.824	10.243	90.811	1.00	20.00
ATOM	1018	C	PHE	126	36.313	6.375	86.337	1.00	20.00
ATOM	1019	O	PHE	126	35.314	6.051	85.695	1.00	20.00
ATOM	1020	N	SER	127	37.491	5.752	86.157	1.00	20.00
ATOM	1021	CA	SER	127	37.559	4.790	85.099	1.00	20.00
ATOM	1022	CB	SER	127	38.463	5.222	83.931	1.00	20.00
ATOM	1023	OG	SER	127	39.823	5.213	84.338	1.00	20.00
ATOM	1024	C	SER	127	38.093	3.484	85.593	1.00	20.00
ATOM	1025	O	SER	127	38.762	3.399	86.622	1.00	20.00
ATOM	1026	N	ASN	128	37.773	2.419	84.830	1.00	20.00
ATOM	1027	CA	ASN	128	38.272	1.090	85.056	1.00	20.00
ATOM	1028	CB	ASN	128	39.735	0.895	84.611	1.00	20.00
ATOM	1029	CG	ASN	128	39.832	1.046	83.097	1.00	20.00
ATOM	1030	OD1	ASN	128	40.440	1.995	82.604	1.00	20.00
ATOM	1031	ND2	ASN	128	39.233	0.089	82.337	1.00	20.00
ATOM	1032	C	ASN	128	38.197	0.700	86.497	1.00	20.00
ATOM	1033	O	ASN	128	39.228	0.550	87.153	1.00	20.00
ATOM	1034	N	ASN	129	36.977	0.539	87.046	1.00	20.00
ATOM	1035	CA	ASN	129	36.919	0.066	88.402	1.00	20.00
ATOM	1036	CB	ASN	129	36.561	1.183	89.392	1.00	20.00
ATOM	1037	CG	ASN	129	37.695	2.197	89.570	1.00	20.00
ATOM	1038	OD1	ASN	129	38.830	1.889	89.731	1.00	20.00
ATOM	1039	ND2	ASN	129	37.381	3.442	88.922	1.00	20.00
ATOM	1040	C	ASN	129	35.824	-0.953	88.478	1.00	20.00
ATOM	1041	O	ASN	129	34.736	-0.657	88.969	1.00	20.00
ATOM	1042	N	PRO	130	36.113	-2.167	88.094	1.00	20.00
ATOM	1043	CA	PRO	130	35.133	-3.218	87.967	1.00	20.00
ATOM	1044	CD	PRO	130	37.477	-2.650	87.977	1.00	20.00
ATOM	1045	CB	PRO	130	35.928	-4.509	87.765	1.00	20.00
ATOM	1046	CG	PRO	130	37.329	-4.036	87.927	1.00	20.00
ATOM	1047	C	PRO	130	34.166	-3.318	89.118	1.00	20.00
ATOM	1048	O	PRO	130	32.965	-3.409	88.870	1.00	20.00
ATOM	1049	N	ALA	131	34.670	-3.327	90.365	1.00	20.00
ATOM	1050	CA	ALA	131	33.926	-3.463	91.592	1.00	20.00
ATOM	1051	CB	ALA	131	34.809	-3.930	92.762	1.00	20.00
ATOM	1052	C	ALA	131	33.247	-2.196	92.065	1.00	20.00
ATOM	1053	O	ALA	131	32.352	-2.253	92.884	1.00	20.00
ATOM	1054	N	LEU	132	33.686	-1.015	91.574	1.00	20.00
ATOM	1055	CA	LEU	132	33.213	0.222	92.140	1.00	20.00
ATOM	1056	CB	LEU	132	33.939	1.453	91.558	1.00	20.00
ATOM	1057	CG	LEU	132	33.469	2.799	92.139	1.00	20.00
ATOM	1058	CD1	LEU	132	33.739	2.881	93.647	1.00	20.00
ATOM	1059	CD2	LEU	132	34.091	3.978	91.369	1.00	20.00
ATOM	1060	C	LEU	132	31.745	0.413	91.960	1.00	20.00
ATOM	1061	O	LEU	132	31.198	0.282	90.868	1.00	20.00
ATOM	1062	N	CYS	133	31.068	0.757	93.071	1.00	20.00
ATOM	1063	CA	CYS	133	29.663	0.994	93.024	1.00	20.00
ATOM	1064	CB	CYS	133	28.845	-0.167	93.563	1.00	20.00
ATOM	1065	SG	CYS	133	28.793	-1.500	92.338	1.00	20.00
ATOM	1066	C	CYS	133	29.389	2.230	93.814	1.00	20.00
ATOM	1067	O	CYS	133	30.309	2.967	94.165	1.00	20.00
ATOM	1068	N	ASN	134	28.102	2.508	94.085	1.00	20.00
ATOM	1069	CA	ASN	134	27.765	3.698	94.803	1.00	20.00
ATOM	1070	CB	ASN	134	28.367	3.735	96.219	1.00	20.00
ATOM	1071	CG	ASN	134	27.653	2.690	97.066	1.00	20.00
ATOM	1072	OD1	ASN	134	26.570	2.936	97.593	1.00	20.00
ATOM	1073	ND2	ASN	134	28.273	1.486	97.198	1.00	20.00
ATOM	1074	C	ASN	134	28.325	4.848	94.026	1.00	20.00
ATOM	1075	O	ASN	134	28.806	5.818	94.610	1.00	20.00
ATOM	1076	N	VAL	135	28.441	4.664	92.693	1.00	20.00
ATOM	1077	CA	VAL	135	28.828	5.679	91.749	1.00	20.00
ATOM	1078	CB	VAL	135	29.541	5.104	90.561	1.00	20.00

Figure 6 (continued)

ATOM	1079	CG1	VAL	135	29.869	6.247	89.585	1.00	20.00
ATOM	1080	CG2	VAL	135	30.775	4.333	91.058	1.00	20.00
ATOM	1081	C	VAL	135	27.661	6.465	91.212	1.00	20.00
ATOM	1082	O	VAL	135	27.725	7.687	91.089	1.00	20.00
ATOM	1083	N	GLU	136	26.569	5.750	90.849	1.00	20.00
ATOM	1084	CA	GLU	136	25.403	6.303	90.197	1.00	20.00
ATOM	1085	CB	GLU	136	24.397	5.239	89.724	1.00	20.00
ATOM	1086	CG	GLU	136	24.872	4.364	88.564	1.00	20.00
ATOM	1087	CD	GLU	136	23.716	3.638	88.207	1.00	20.00
ATOM	1088	OE1	GLU	136	22.685	3.964	87.773	1.00	20.00
ATOM	1089	OE2	GLU	136	23.871	2.199	88.372	1.00	20.00
ATOM	1090	C	GLU	136	24.646	7.159	91.248	1.00	20.00
ATOM	1091	O	GLU	136	23.956	8.096	90.754	1.00	20.00
ATOM	1092	N	SER	137	24.750	6.798	92.430	1.00	20.00
ATOM	1093	CA	SER	137	24.071	7.350	93.560	1.00	20.00
ATOM	1094	CB	SER	137	24.290	6.481	94.807	1.00	20.00
ATOM	1095	OG	SER	137	25.680	6.249	94.980	1.00	20.00
ATOM	1096	C	SER	137	24.503	8.753	93.871	1.00	20.00
ATOM	1097	O	SER	137	23.834	9.423	94.684	1.00	20.00
ATOM	1098	N	ILE	138	25.647	9.232	93.345	1.00	20.00
ATOM	1099	CA	ILE	138	26.094	10.544	93.733	1.00	20.00
ATOM	1100	CB	ILE	138	27.582	10.629	93.900	1.00	20.00
ATOM	1101	CG2	ILE	138	27.945	12.095	94.188	1.00	20.00
ATOM	1102	CG1	ILE	138	28.055	9.647	94.982	1.00	20.00
ATOM	1103	CD1	ILE	138	29.563	9.414	94.969	1.00	20.00
ATOM	1104	C	ILE	138	25.724	11.579	92.710	1.00	20.00
ATOM	1105	O	ILE	138	25.821	11.357	91.503	1.00	20.00
ATOM	1106	N	GLN	139	25.288	12.764	93.192	1.00	20.00
ATOM	1107	CA	GLN	139	24.929	13.831	92.306	1.00	20.00
ATOM	1108	CB	GLN	139	23.652	14.566	92.754	1.00	20.00
ATOM	1109	CG	GLN	139	23.092	15.539	91.716	1.00	20.00
ATOM	1110	CD	GLN	139	21.688	15.926	92.161	1.00	20.00
ATOM	1111	OE1	GLN	139	21.024	16.749	91.532	1.00	20.00
ATOM	1112	NE2	GLN	139	21.216	15.308	93.277	1.00	20.00
ATOM	1113	C	GLN	139	26.075	14.794	92.284	1.00	20.00
ATOM	1114	O	GLN	139	26.160	15.724	93.086	1.00	20.00
ATOM	1115	N	TRP	140	26.977	14.597	91.309	1.00	20.00
ATOM	1116	CA	TRP	140	28.180	15.363	91.161	1.00	20.00
ATOM	1117	CB	TRP	140	29.163	14.778	90.137	1.00	20.00
ATOM	1118	CG	TRP	140	29.818	13.522	90.633	1.00	20.00
ATOM	1119	CD2	TRP	140	30.821	13.520	91.679	1.00	20.00
ATOM	1120	CD1	TRP	140	29.592	12.217	90.330	1.00	20.00
ATOM	1121	NE1	TRP	140	30.396	11.400	91.091	1.00	20.00
ATOM	1122	CE2	TRP	140	31.156	12.191	91.927	1.00	20.00
ATOM	1123	CE3	TRP	140	31.410	14.545	92.364	1.00	20.00
ATOM	1124	CZ2	TRP	140	32.090	11.863	92.869	1.00	20.00
ATOM	1125	CZ3	TRP	140	32.355	14.211	93.308	1.00	20.00
ATOM	1126	CH2	TRP	140	32.688	12.896	93.555	1.00	20.00
ATOM	1127	C	TRP	140	27.853	16.764	90.784	1.00	20.00
ATOM	1128	O	TRP	140	28.699	17.646	90.889	1.00	20.00
ATOM	1129	N	ARG	141	26.637	17.008	90.276	1.00	20.00
ATOM	1130	CA	ARG	141	26.301	18.348	89.897	1.00	20.00
ATOM	1131	CB	ARG	141	24.877	18.417	89.325	1.00	20.00
ATOM	1132	CG	ARG	141	24.516	19.908	88.917	1.00	20.00
ATOM	1133	CD	ARG	141	23.284	20.001	88.031	1.00	20.00
ATOM	1134	NE	ARG	141	22.103	19.536	88.789	1.00	20.00
ATOM	1135	CZ	ARG	141	21.404	20.418	89.561	1.00	20.00
ATOM	1136	NH1	ARG	141	21.799	21.722	89.638	1.00	20.00
ATOM	1137	NH2	ARG	141	20.305	19.998	90.253	1.00	20.00
ATOM	1138	C	ARG	141	26.410	19.219	91.109	1.00	20.00
ATOM	1139	O	ARG	141	26.800	20.381	91.011	1.00	20.00
ATOM	1140	N	ASP	142	26.040	18.695	92.292	1.00	20.00
ATOM	1141	CA	ASP	142	26.142	19.491	93.480	1.00	20.00
ATOM	1142	CB	ASP	142	25.567	18.779	94.715	1.00	20.00
ATOM	1143	CG	ASP	142	24.056	18.687	94.652	1.00	20.00
ATOM	1144	OD1	ASP	142	23.505	19.441	93.706	1.00	20.00
ATOM	1145	OD2	ASP	142	23.432	17.860	95.270	1.00	20.00
ATOM	1146	C	ASP	142	27.580	19.782	93.766	1.00	20.00
ATOM	1147	O	ASP	142	27.964	20.923	94.034	1.00	20.00
ATOM	1148	N	ILE	143	28.443	18.743	93.726	1.00	20.00
ATOM	1149	CA	ILE	143	29.832	18.901	94.069	1.00	20.00
ATOM	1150	CB	ILE	143	30.527	17.584	94.220	1.00	20.00
ATOM	1151	CG2	ILE	143	32.013	17.861	94.496	1.00	20.00
ATOM	1152	CG1	ILE	143	29.841	16.766	95.327	1.00	20.00
ATOM	1153	CD1	ILE	143	30.264	15.299	95.362	1.00	20.00
ATOM	1154	C	ILE	143	30.563	19.713	93.049	1.00	20.00
ATOM	1155	O	ILE	143	31.338	20.615	93.409	1.00	20.00

Figure 6 (continued)

ATOM	1156	N	VAL	144	30.393	19.425	91.746	1.00	20.00
ATOM	1157	CA	VAL	144	31.124	20.114	90.716	1.00	20.00
ATOM	1158	CB	VAL	144	31.795	19.194	89.741	1.00	20.00
ATOM	1159	CG1	VAL	144	32.648	18.362	90.491	1.00	20.00
ATOM	1160	CG2	VAL	144	30.714	18.350	89.046	1.00	20.00
ATOM	1161	C	VAL	144	30.141	20.931	89.943	1.00	20.00
ATOM	1162	O	VAL	144	28.999	20.521	89.760	1.00	20.00
ATOM	1163	N	SER	145	30.563	22.110	89.449	1.00	40.00
ATOM	1164	CA	SER	145	29.643	22.943	88.732	1.00	40.00
ATOM	1165	CB	SER	145	30.257	24.249	88.196	1.00	40.00
ATOM	1166	OG	SER	145	30.673	25.071	89.276	1.00	40.00
ATOM	1167	C	SER	145	29.123	22.163	87.570	1.00	40.00
ATOM	1168	O	SER	145	29.739	21.194	87.131	1.00	40.00
ATOM	1169	N	SER	146	27.961	22.580	87.055	1.00	40.00
ATOM	1170	CA	SER	146	27.292	21.887	85.989	1.00	40.00
ATOM	1171	CB	SER	146	26.000	22.586	85.532	1.00	40.00
ATOM	1172	OG	SER	146	26.304	23.856	84.973	1.00	40.00
ATOM	1173	C	SER	146	28.217	21.046	84.824	1.00	40.00
ATOM	1174	O	SER	146	28.314	20.832	84.134	1.00	40.00
ATOM	1175	N	ASP	147	28.939	22.952	84.583	1.00	40.00
ATOM	1176	CA	ASP	147	29.847	22.975	83.480	1.00	40.00
ATOM	1177	CB	ASP	147	30.636	24.292	83.305	1.00	40.00
ATOM	1178	CG	ASP	147	31.479	24.285	82.086	1.00	40.00
ATOM	1179	OD1	ASP	147	31.400	23.245	81.376	1.00	40.00
ATOM	1180	OD2	ASP	147	32.078	25.324	81.786	1.00	40.00
ATOM	1181	C	ASP	147	30.821	21.874	83.729	1.00	40.00
ATOM	1182	O	ASP	147	31.224	21.159	82.815	1.00	40.00
ATOM	1183	N	PHE	148	31.212	21.701	85.001	1.00	40.00
ATOM	1184	CA	PHE	148	32.146	20.677	85.353	1.00	40.00
ATOM	1185	CB	PHE	148	32.866	20.717	86.831	1.00	40.00
ATOM	1186	CG	PHE	148	33.413	21.930	87.007	1.00	40.00
ATOM	1187	CD1	PHE	148	34.745	21.906	86.662	1.00	40.00
ATOM	1188	CD2	PHE	148	32.881	23.090	87.517	1.00	40.00
ATOM	1189	CE1	PHE	148	35.550	23.023	86.821	1.00	40.00
ATOM	1190	CE2	PHE	148	33.661	24.211	87.679	1.00	40.00
ATOM	1191	CZ	PHE	148	34.989	24.179	87.330	1.00	40.00
ATOM	1192	C	PHE	148	31.548	19.337	85.076	1.00	40.00
ATOM	1193	O	PHE	148	32.255	18.412	84.685	1.00	40.00
ATOM	1194	N	LEU	149	30.218	19.180	85.259	1.00	40.00
ATOM	1195	CA	LEU	149	29.675	17.858	85.078	1.00	40.00
ATOM	1196	CB	LEU	149	28.154	17.741	85.313	1.00	40.00
ATOM	1197	CG	LEU	149	27.699	17.793	86.785	1.00	40.00
ATOM	1198	CD1	LEU	149	27.904	19.177	87.411	1.00	40.00
ATOM	1199	CD2	LEU	149	26.256	17.287	86.954	1.00	40.00
ATOM	1200	C	LEU	149	29.918	17.376	83.683	1.00	40.00
ATOM	1201	O	LEU	149	30.200	16.196	83.472	1.00	40.00
ATOM	1202	N	SER	150	29.837	18.269	82.687	1.00	40.00
ATOM	1203	CA	SER	150	29.984	17.863	81.326	1.00	40.00
ATOM	1204	CB	SER	150	29.921	19.017	80.335	1.00	40.00
ATOM	1205	OG	SER	150	30.998	19.913	80.574	1.00	40.00
ATOM	1206	C	SER	150	31.315	17.175	81.149	1.00	40.00
ATOM	1207	O	SER	150	31.425	16.176	80.440	1.00	40.00
ATOM	1208	N	ASN	151	32.360	17.717	81.799	1.00	40.00
ATOM	1209	CA	ASN	151	33.712	17.251	81.665	1.00	40.00
ATOM	1210	CB	ASN	151	34.724	18.153	82.390	1.00	40.00
ATOM	1211	CG	ASN	151	34.738	19.612	81.765	1.00	40.00
ATOM	1212	OD1	ASN	151	34.014	19.746	80.739	1.00	40.00
ATOM	1213	ND2	ASN	151	35.596	20.435	82.216	1.00	40.00
ATOM	1214	C	ASN	151	33.889	16.871	82.230	1.00	40.00
ATOM	1215	O	ASN	151	34.722	15.108	81.740	1.00	40.00
ATOM	1216	N	MET	152	33.128	15.513	83.283	1.00	40.00
ATOM	1217	CA	MET	152	33.330	14.269	83.982	1.00	40.00
ATOM	1218	CB	MET	152	32.253	14.010	85.050	1.00	40.00
ATOM	1219	CG	MET	152	32.593	12.883	86.026	1.00	40.00
ATOM	1220	SD	MET	152	31.367	12.649	87.348	1.00	40.00
ATOM	1221	CE	MET	152	31.655	14.266	88.127	1.00	40.00
ATOM	1222	C	MET	152	33.343	13.121	83.026	1.00	40.00
ATOM	1223	O	MET	152	32.474	12.997	82.165	1.00	40.00
ATOM	1224	N	SER	153	34.368	12.250	83.157	1.00	40.00
ATOM	1225	CA	SER	153	34.471	11.123	82.280	1.00	40.00
ATOM	1226	CB	SER	153	35.786	11.081	81.483	1.00	40.00
ATOM	1227	OG	SER	153	35.840	12.177	80.581	1.00	40.00
ATOM	1228	C	SER	153	34.405	9.877	83.094	1.00	40.00
ATOM	1229	O	SER	153	35.285	9.594	83.907	1.00	40.00
ATOM	1230	N	MET	154	33.333	9.093	82.893	1.00	40.00
ATOM	1231	CA	MET	154	33.230	7.859	83.601	1.00	40.00
ATOM	1232	CB	MET	154	31.968	7.749	84.462	1.00	40.00

Figure 6 (continued)

ATOM	1233	CG	MET	154	31.991	8.700	85.662	1.00	40.00
ATOM	1234	SD	MET	154	30.442	8.786	86.607	1.00	40.00
ATOM	1235	CE	MET	154	29.667	10.012	85.513	1.00	40.00
ATOM	1236	C	MET	154	33.215	6.783	82.577	1.00	40.00
ATOM	1237	O	MET	154	32.267	6.665	81.802	1.00	40.00
ATOM	1238	N	ASP	155	34.283	5.969	82.540	1.00	40.00
ATOM	1239	CA	ASP	155	34.292	4.918	81.579	1.00	40.00
ATOM	1240	CB	ASP	155	35.691	4.375	81.243	1.00	40.00
ATOM	1241	CG	ASP	155	35.566	3.514	79.992	1.00	40.00
ATOM	1242	OD1	ASP	155	34.446	3.465	79.417	1.00	40.00
ATOM	1243	OD2	ASP	155	36.590	2.892	79.599	1.00	40.00
ATOM	1244	C	ASP	155	33.519	3.827	82.204	1.00	40.00
ATOM	1245	O	ASP	155	33.697	3.600	83.411	1.00	40.00
ATOM	1246	N	PHE	156	32.731	3.114	81.370	1.00	40.00
ATOM	1247	CA	PHE	156	31.853	2.051	81.774	1.00	40.00
ATOM	1248	CB	PHE	156	31.040	1.483	80.595	1.00	40.00
ATOM	1249	CG	PHE	156	30.123	2.536	80.071	1.00	40.00
ATOM	1250	CD1	PHE	156	30.600	3.548	79.269	1.00	40.00
ATOM	1251	CD2	PHE	156	28.779	2.498	80.364	1.00	40.00
ATOM	1252	CE1	PHE	156	29.753	4.516	78.780	1.00	40.00
ATOM	1253	CE2	PHE	156	27.928	3.462	79.870	1.00	40.00
ATOM	1254	CZ	PHE	156	28.414	4.474	79.086	1.00	40.00
ATOM	1255	C	PHE	156	32.652	0.896	82.298	1.00	40.00
ATOM	1256	O	PHE	156	32.133	-0.214	82.406	1.00	40.00
ATOM	1257	N	GLN	157	33.928	1.172	82.654	1.00	40.00
ATOM	1258	CA	GLN	157	34.682	0.035	83.193	1.00	40.00
ATOM	1259	CB	GLN	157	36.261	0.220	83.147	1.00	40.00
ATOM	1260	CG	GLN	157	36.920	-1.060	83.577	1.00	40.00
ATOM	1261	CD	GLN	157	36.539	-2.155	82.595	1.00	40.00
ATOM	1262	OE1	GLN	157	35.829	-1.905	81.621	1.00	40.00
ATOM	1263	NE2	GLN	157	37.018	-3.400	82.859	1.00	40.00
ATOM	1264	C	GLN	157	34.259	-0.117	84.613	1.00	40.00
ATOM	1265	O	GLN	157	34.691	-1.040	85.298	1.00	40.00
ATOM	1266	N	ASN	158	33.416	0.812	85.106	1.00	40.00
ATOM	1267	CA	ASN	158	32.945	0.694	86.456	1.00	40.00
ATOM	1268	CB	ASN	158	32.249	1.957	86.991	1.00	40.00
ATOM	1269	CG	ASN	158	33.321	3.010	87.232	1.00	40.00
ATOM	1270	OD1	ASN	158	34.482	2.688	87.478	1.00	40.00
ATOM	1271	ND2	ASN	158	32.918	4.307	87.169	1.00	40.00
ATOM	1272	C	ASN	158	31.962	-0.434	86.502	1.00	40.00
ATOM	1273	O	ASN	158	31.713	-1.097	85.497	1.00	40.00
ATOM	1274	N	HIS	159	31.388	-0.692	87.695	1.00	40.00
ATOM	1275	CA	HIS	159	30.496	-1.805	87.868	1.00	40.00
ATOM	1276	ND1	HIS	159	28.560	-3.969	89.855	1.00	40.00
ATOM	1277	NE2	HIS	159	29.574	-5.943	89.508	1.00	40.00
ATOM	1278	CE1	HIS	159	28.425	-5.319	89.694	1.00	40.00
ATOM	1279	CD2	HIS	159	30.498	-4.927	89.342	1.00	40.00
ATOM	1280	CG	HIS	159	29.893	-3.710	89.428	1.00	40.00
ATOM	1281	CB	HIS	159	30.482	-2.337	89.311	1.00	40.00
ATOM	1282	C	HIS	159	29.099	-1.389	87.517	1.00	40.00
ATOM	1283	O	HIS	159	28.816	-0.203	87.352	1.00	40.00
ATOM	1284	N	LEU	160	28.187	-2.379	87.382	1.00	40.00
ATOM	1285	CA	LEU	160	26.814	-2.106	87.060	1.00	40.00
ATOM	1286	CB	LEU	160	26.107	-3.247	86.307	1.00	40.00
ATOM	1287	CG	LEU	160	26.696	-3.508	84.908	1.00	40.00
ATOM	1288	CD1	LEU	160	28.149	-4.000	84.998	1.00	40.00
ATOM	1289	CD2	LEU	160	25.794	-4.442	84.086	1.00	40.00
ATOM	1290	C	LEU	160	26.070	-1.873	88.341	1.00	40.00
ATOM	1291	O	LEU	160	26.472	-2.342	89.403	1.00	40.00
ATOM	1292	N	GLY	161	24.928	-1.164	88.240	1.00	40.00
ATOM	1293	CA	GLY	161	24.107	-0.713	89.334	1.00	40.00
ATOM	1294	C	GLY	161	23.611	-1.861	90.176	1.00	40.00
ATOM	1295	O	GLY	161	22.862	-1.641	91.128	1.00	40.00
ATOM	1296	N	SER	162	24.007	-3.098	89.846	1.00	40.00
ATOM	1297	CA	SER	162	23.573	-4.255	90.554	1.00	40.00
ATOM	1298	CB	SER	162	24.217	-5.543	90.018	1.00	40.00
ATOM	1299	OG	SER	162	25.617	-5.519	90.253	1.00	40.00
ATOM	1300	C	SER	162	23.947	-4.144	92.005	1.00	40.00
ATOM	1301	O	SER	162	23.297	-4.749	92.855	1.00	40.00
ATOM	1302	N	CYS	163	24.998	-3.377	92.347	1.00	20.00
ATOM	1303	CA	CYS	163	25.471	-3.385	93.708	1.00	20.00
ATOM	1304	CB	CYS	163	26.601	-2.412	94.018	1.00	20.00
ATOM	1305	SG	CYS	163	28.216	-3.031	93.499	1.00	20.00
ATOM	1306	C	CYS	163	24.431	-3.146	94.769	1.00	20.00
ATOM	1307	O	CYS	163	24.256	-4.027	95.603	1.00	20.00
ATOM	1308	N	GLN	164	23.706	-2.003	94.826	1.00	40.00
ATOM	1309	CA	GLN	164	22.859	-1.898	95.996	1.00	40.00

Figure 6 (continued)

ATOM	1310	CB	GLN	164	23.611	-1.447	97.263	1.00	40.00
ATOM	1311	CG	GLN	164	24.612	-2.460	97.823	1.00	40.00
ATOM	1312	CD	GLN	164	25.256	-1.849	99.059	1.00	40.00
ATOM	1313	OE1	GLN	164	25.834	-0.765	98.997	1.00	40.00
ATOM	1314	NE2	GLN	164	25.155	-2.558	100.216	1.00	40.00
ATOM	1315	C	GLN	164	21.763	-0.888	95.825	1.00	40.00
ATOM	1316	O	GLN	164	21.240	-0.579	94.732	1.00	40.00
ATOM	1317	N	LYS	165	21.374	-0.272	96.971	1.00	40.00
ATOM	1318	CA	LYS	165	20.320	0.702	97.072	1.00	40.00
ATOM	1319	CB	LYS	165	18.957	0.054	97.384	1.00	40.00
ATOM	1320	CG	LYS	165	17.794	1.038	97.503	1.00	40.00
ATOM	1321	CD	LYS	165	16.420	0.361	97.435	1.00	40.00
ATOM	1322	CE	LYS	165	16.216	-0.741	98.479	1.00	40.00
ATOM	1323	NZ	LYS	165	15.818	-0.147	99.775	1.00	40.00
ATOM	1324	C	LYS	165	20.660	1.625	98.213	1.00	40.00
ATOM	1325	O	LYS	165	21.489	1.293	99.058	1.00	40.00
ATOM	1326	N	CYS	166	20.032	2.823	98.262	1.00	20.00
ATOM	1327	CA	CYS	166	20.299	3.762	99.324	1.00	20.00
ATOM	1328	CB	CYS	166	20.295	5.252	98.901	1.00	20.00
ATOM	1329	SG	CYS	166	21.577	5.745	97.700	1.00	20.00
ATOM	1330	C	CYS	166	19.219	3.620	100.350	1.00	20.00
ATOM	1331	O	CYS	166	18.356	2.750	100.247	1.00	20.00
ATOM	1332	N	ASP	167	19.264	4.490	101.391	1.00	20.00
ATOM	1333	CA	ASP	167	18.286	4.447	102.442	1.00	20.00
ATOM	1334	CB	ASP	167	18.787	5.021	103.777	1.00	20.00
ATOM	1335	CG	ASP	167	19.866	4.096	104.320	1.00	20.00
ATOM	1336	OD1	ASP	167	20.212	3.110	103.616	1.00	20.00
ATOM	1337	OD2	ASP	167	20.357	4.362	105.450	1.00	20.00
ATOM	1338	C	ASP	167	17.120	5.283	102.017	1.00	20.00
ATOM	1339	O	ASP	167	17.221	6.116	101.119	1.00	20.00
ATOM	1340	N	PRO	168	15.994	5.035	102.630	1.00	20.00
ATOM	1341	CA	PRO	168	14.801	5.792	102.377	1.00	20.00
ATOM	1342	CD	PRO	168	15.722	3.769	103.285	1.00	20.00
ATOM	1343	CB	PRO	168	13.657	5.005	103.019	1.00	20.00
ATOM	1344	CG	PRO	168	14.352	3.987	103.945	1.00	20.00
ATOM	1345	C	PRO	168	14.980	7.169	102.929	1.00	20.00
ATOM	1346	O	PRO	168	14.295	8.089	102.485	1.00	20.00
ATOM	1347	N	SER	169	15.883	7.319	103.915	1.00	20.00
ATOM	1348	CA	SER	169	16.143	8.581	104.541	1.00	20.00
ATOM	1349	CB	SER	169	17.050	8.455	105.749	1.00	20.00
ATOM	1350	OG	SER	169	17.314	9.731	106.332	1.00	20.00
ATOM	1351	C	SER	169	16.799	9.493	103.555	1.00	20.00
ATOM	1352	O	SER	169	16.481	10.673	103.488	1.00	20.00
ATOM	1353	N	CYS	170	17.724	8.950	102.741	1.00	20.00
ATOM	1354	CA	CYS	170	18.471	9.781	101.844	1.00	20.00
ATOM	1355	CB	CYS	170	19.480	9.021	100.964	1.00	20.00
ATOM	1356	SG	CYS	170	20.686	8.015	101.878	1.00	20.00
ATOM	1357	C	CYS	170	17.520	10.444	100.903	1.00	20.00
ATOM	1358	O	CYS	170	16.343	10.101	100.801	1.00	20.00
ATOM	1359	N	PRO	171	18.052	11.433	100.240	1.00	20.00
ATOM	1360	CA	PRO	171	17.297	12.152	99.251	1.00	20.00
ATOM	1361	CD	PRO	171	19.025	12.292	100.897	1.00	20.00
ATOM	1362	CB	PRO	171	18.056	13.451	99.001	1.00	20.00
ATOM	1363	CG	PRO	171	18.791	13.702	100.328	1.00	20.00
ATOM	1364	C	PRO	171	17.159	11.284	98.040	1.00	20.00
ATOM	1365	O	PRO	171	17.841	10.274	97.962	1.00	20.00
ATOM	1366	N	ASN	172	16.288	11.695	97.094	1.00	20.00
ATOM	1367	CA	ASN	172	15.986	10.933	95.916	1.00	20.00
ATOM	1368	CB	ASN	172	15.258	11.749	94.829	1.00	20.00
ATOM	1369	CG	ASN	172	13.881	12.072	95.309	1.00	20.00
ATOM	1370	OD1	ASN	172	13.402	11.580	96.343	1.00	20.00
ATOM	1371	ND2	ASN	172	13.128	12.919	94.529	1.00	20.00
ATOM	1372	C	ASN	172	17.228	10.384	95.289	1.00	20.00
ATOM	1373	O	ASN	172	17.903	11.060	94.514	1.00	20.00
ATOM	1374	N	GLY	173	17.558	9.125	95.632	1.00	20.00
ATOM	1375	CA	GLY	173	18.622	8.401	95.000	1.00	20.00
ATOM	1376	C	GLY	173	19.947	9.070	95.177	1.00	20.00
ATOM	1377	O	GLY	173	20.756	9.062	94.251	1.00	20.00
ATOM	1378	N	SER	174	20.232	9.681	96.342	1.00	20.00
ATOM	1379	CA	SER	174	21.547	10.255	96.421	1.00	20.00
ATOM	1380	CB	SER	174	21.547	11.791	96.495	1.00	20.00
ATOM	1381	OG	SER	174	20.948	12.223	97.709	1.00	20.00
ATOM	1382	C	SER	174	22.229	9.761	97.659	1.00	20.00
ATOM	1383	O	SER	174	21.762	10.012	98.768	1.00	20.00
ATOM	1384	N	CYS	175	23.350	9.024	97.506	1.00	20.00
ATOM	1385	CA	CYS	175	24.068	8.612	98.680	1.00	20.00
ATOM	1386	CB	CYS	175	23.349	7.514	99.504	1.00	20.00

Figure 6 (continued)

ATOM	1387	SG	CYS	175	23.313	5.847	98.761	1.00	20.00
ATOM	1388	C	CYS	175	25.416	8.102	98.273	1.00	20.00
ATOM	1389	O	CYS	175	25.587	7.585	97.173	1.00	20.00
ATOM	1390	N	TRP	176	26.428	8.289	99.144	1.00	20.00
ATOM	1391	CA	TRP	176	27.758	7.808	98.885	1.00	20.00
ATOM	1392	CB	TRP	176	28.811	8.464	99.795	1.00	20.00
ATOM	1393	CG	TRP	176	28.970	9.942	99.510	1.00	20.00
ATOM	1394	CD2	TRP	176	29.858	10.492	98.522	1.00	20.00
ATOM	1395	CD1	TRP	176	28.324	11.001	100.077	1.00	20.00
ATOM	1396	NE1	TRP	176	28.752	12.176	99.505	1.00	20.00
ATOM	1397	CE2	TRP	176	29.697	11.877	98.547	1.00	20.00
ATOM	1398	CE3	TRP	176	30.737	9.892	97.666	1.00	20.00
ATOM	1399	CZ2	TRP	176	30.412	12.687	97.709	1.00	20.00
ATOM	1400	CZ3	TRP	176	31.457	10.710	96.823	1.00	20.00
ATOM	1401	CH2	TRP	176	31.296	12.080	96.843	1.00	20.00
ATOM	1402	C	TRP	176	27.786	6.323	99.068	1.00	20.00
ATOM	1403	O	TRP	176	28.502	5.609	98.366	1.00	20.00
ATOM	1404	N	GLY	177	27.009	5.824	100.048	1.00	20.00
ATOM	1405	CA	GLY	177	26.932	4.416	100.312	1.00	20.00
ATOM	1406	C	GLY	177	25.598	4.198	100.945	1.00	20.00
ATOM	1407	O	GLY	177	24.833	5.142	101.132	1.00	20.00
ATOM	1408	N	ALA	178	25.256	2.939	101.274	1.00	20.00
ATOM	1409	CA	ALA	178	23.995	2.740	101.918	1.00	20.00
ATOM	1410	CB	ALA	178	23.463	1.300	101.813	1.00	20.00
ATOM	1411	C	ALA	178	24.195	3.049	103.365	1.00	20.00
ATOM	1412	O	ALA	178	25.186	2.558	103.978	1.00	20.00
ATOM	1413	N	GLY	179	23.291	3.858	103.950	1.00	20.00
ATOM	1414	CA	GLY	179	23.422	4.184	105.341	1.00	20.00
ATOM	1415	C	GLY	179	22.916	5.577	105.537	1.00	20.00
ATOM	1416	O	GLY	179	22.867	6.374	104.602	1.00	20.00
ATOM	1417	N	GLU	180	22.525	5.898	106.785	1.00	20.00
ATOM	1418	CA	GLU	180	22.012	7.195	107.111	1.00	20.00
ATOM	1419	CB	GLU	180	21.604	7.297	108.592	1.00	20.00
ATOM	1420	CG	GLU	180	20.414	6.415	108.976	1.00	20.00
ATOM	1421	CD	GLU	180	19.136	7.190	108.693	1.00	20.00
ATOM	1422	OE1	GLU	180	19.242	8.369	108.261	1.00	20.00
ATOM	1423	OE2	GLU	180	18.035	6.616	108.912	1.00	20.00
ATOM	1424	C	GLU	180	23.103	8.195	106.903	1.00	20.00
ATOM	1425	O	GLU	180	22.905	9.235	106.277	1.00	20.00
ATOM	1426	N	GLU	181	24.299	7.882	107.431	1.00	20.00
ATOM	1427	CA	GLU	181	25.443	8.746	107.365	1.00	20.00
ATOM	1428	CB	GLU	181	26.633	8.195	108.170	1.00	20.00
ATOM	1429	CG	GLU	181	27.875	9.086	108.136	1.00	20.00
ATOM	1430	CD	GLU	181	28.952	8.409	108.973	1.00	20.00
ATOM	1431	OE1	GLU	181	28.646	7.352	109.586	1.00	20.00
ATOM	1432	OE2	GLU	181	30.095	8.939	109.009	1.00	20.00
ATOM	1433	C	GLU	181	25.889	8.860	105.945	1.00	20.00
ATOM	1434	O	GLU	181	26.311	9.922	105.492	1.00	20.00
ATOM	1435	N	ASN	182	25.780	7.746	105.206	1.00	20.00
ATOM	1436	CA	ASN	182	26.275	7.631	103.869	1.00	20.00
ATOM	1437	CB	ASN	182	26.103	6.214	103.305	1.00	20.00
ATOM	1438	CG	ASN	182	27.010	5.283	104.099	1.00	20.00
ATOM	1439	OD1	ASN	182	26.768	5.014	105.275	1.00	20.00
ATOM	1440	ND2	ASN	182	28.084	4.772	103.440	1.00	20.00
ATOM	1441	C	ASN	182	25.580	8.593	102.956	1.00	20.00
ATOM	1442	O	ASN	182	26.177	9.028	101.972	1.00	20.00
ATOM	1443	N	CYS	183	24.305	8.930	103.248	1.00	20.00
ATOM	1444	CA	CYS	183	23.517	9.796	102.409	1.00	20.00
ATOM	1445	CB	CYS	183	22.234	10.333	103.070	1.00	20.00
ATOM	1446	SG	CYS	183	21.041	9.063	103.574	1.00	20.00
ATOM	1447	C	CYS	183	24.299	11.001	102.038	1.00	20.00
ATOM	1448	O	CYS	183	25.111	11.502	102.813	1.00	20.00
ATOM	1449	N	GLN	184	24.122	11.429	100.774	1.00	40.00
ATOM	1450	CA	GLN	184	24.817	12.571	100.279	1.00	40.00
ATOM	1451	CB	GLN	184	24.808	12.622	98.740	1.00	40.00
ATOM	1452	CG	GLN	184	25.536	13.826	98.143	1.00	40.00
ATOM	1453	CD	GLN	184	25.427	13.713	96.628	1.00	40.00
ATOM	1454	OE1	GLN	184	24.768	12.810	96.113	1.00	40.00
ATOM	1455	NE2	GLN	184	26.092	14.644	95.894	1.00	40.00
ATOM	1456	C	GLN	184	24.042	13.729	100.785	1.00	40.00
ATOM	1457	O	GLN	184	23.545	14.554	100.020	1.00	40.00
ATOM	1458	N	LYS	185	23.937	13.801	102.122	1.00	60.00
ATOM	1459	CA	LYS	185	23.193	14.825	102.782	1.00	60.00
ATOM	1460	CB	LYS	185	23.129	14.586	104.302	1.00	60.00
ATOM	1461	CG	LYS	185	22.030	15.362	105.034	1.00	60.00
ATOM	1462	CD	LYS	185	21.760	14.828	106.444	1.00	60.00
ATOM	1463	CE	LYS	185	21.242	13.386	106.463	1.00	60.00

Figure 6 (continued)

ATOM	1464	NZ	LYS	185	21.056	12.921	107.859	1.00	60.00
ATOM	1465	C	LYS	185	23.892	16.116	102.525	1.00	60.00
ATOM	1466	O	LYS	185	23.262	17.147	102.293	1.00	60.00
ATOM	1467	N	LEU	186	25.235	16.088	102.550	1.00	60.00
ATOM	1468	CA	LEU	186	25.946	17.314	102.380	1.00	60.00
ATOM	1469	CB	LEU	186	27.228	17.377	103.228	1.00	60.00
ATOM	1470	CG	LEU	186	26.966	17.331	104.746	1.00	60.00
ATOM	1471	CD1	LEU	186	26.349	15.985	105.164	1.00	60.00
ATOM	1472	CD2	LEU	186	28.230	17.685	105.546	1.00	60.00
ATOM	1473	C	LEU	186	26.344	17.473	100.947	1.00	60.00
ATOM	1474	O	LEU	186	27.267	16.817	100.466	1.00	60.00
ATOM	1475	N	THR	187	25.637	18.36b	100.226	1.00	60.00
ATOM	1476	CA	THR	187	25.998	18.719	98.864	1.00	60.00
ATOM	1477	CB	THR	187	25.061	18.234	97.815	1.00	60.00
ATOM	1478	OG1	THR	187	23.785	18.834	97.970	1.00	60.00
ATOM	1479	CG2	THR	187	24.947	16.708	97.901	1.00	60.00
ATOM	1480	C	THR	187	25.944	20.230	98.893	1.00	60.00
ATOM	1481	O	THR	187	25.146	20.793	99.625	1.00	60.00
ATOM	1482	N	LYS	188	26.808	20.883	98.111	1.00	60.00
ATOM	1483	CA	LYS	188	26.824	22.312	98.227	1.00	60.00
ATOM	1484	CB	LYS	188	27.940	22.992	97.410	1.00	60.00
ATOM	1485	CG	LYS	188	27.754	22.935	95.892	1.00	60.00
ATOM	1486	CD	LYS	188	28.687	23.881	95.133	1.00	60.00
ATOM	1487	CE	LYS	188	28.505	23.842	93.615	1.00	60.00
ATOM	1488	NZ	LYS	188	27.288	24.596	93.239	1.00	60.00
ATOM	1489	C	LYS	188	25.520	22.666	97.766	1.00	60.00
ATOM	1490	O	LYS	188	24.898	23.672	98.457	1.00	60.00
ATOM	1491	N	ILE	189	25.062	22.432	96.580	1.00	60.00
ATOM	1492	CA	ILE	189	23.844	22.955	96.045	1.00	60.00
ATOM	1493	CB	ILE	189	23.578	22.493	94.642	1.00	60.00
ATOM	1494	CG2	ILE	189	22.174	22.972	94.235	1.00	60.00
ATOM	1495	CG1	ILE	189	24.696	22.988	93.709	1.00	60.00
ATOM	1496	CD1	ILE	189	24.675	22.336	92.327	1.00	60.00
ATOM	1497	C	ILE	189	22.706	22.515	96.898	1.00	60.00
ATOM	1498	O	ILE	189	21.809	23.302	97.202	1.00	60.00
ATOM	1499	N	ILE	190	22.712	21.239	97.328	1.00	60.00
ATOM	1500	CA	ILE	190	21.571	20.792	98.061	1.00	60.00
ATOM	1501	CB	ILE	190	21.090	19.429	97.664	1.00	60.00
ATOM	1502	CG2	ILE	190	19.977	19.021	98.641	1.00	60.00
ATOM	1503	CG1	ILE	190	20.662	19.425	96.187	1.00	60.00
ATOM	1504	CD1	ILE	190	19.540	20.416	95.841	1.00	60.00
ATOM	1505	C	ILE	190	21.662	20.750	99.521	1.00	60.00
ATOM	1506	O	ILE	190	22.747	20.640	99.995	1.00	60.00
ATOM	1507	N	CYS	191	21.072	21.539	100.263	1.00	20.00
ATOM	1508	CA	CYS	191	21.065	21.609	101.689	1.00	20.00
ATOM	1509	CB	CYS	191	22.170	22.473	102.340	1.00	20.00
ATOM	1510	SG	CYS	191	22.159	22.254	104.150	1.00	20.00
ATOM	1511	C	CYS	191	19.747	22.242	101.948	1.00	20.00
ATOM	1512	O	CYS	191	18.784	21.964	101.234	1.00	20.00
ATOM	1513	N	ALA	192	19.636	23.097	102.974	1.00	20.00
ATOM	1514	CA	ALA	192	18.346	23.706	103.116	1.00	20.00
ATOM	1515	CB	ALA	192	18.227	24.618	104.346	1.00	20.00
ATOM	1516	C	ALA	192	18.198	24.559	101.897	1.00	20.00
ATOM	1517	O	ALA	192	19.183	25.063	101.361	1.00	20.00
ATOM	1518	N	GLN	193	16.957	24.733	101.411	1.00	20.00
ATOM	1519	CA	GLN	193	16.750	25.493	100.215	1.00	20.00
ATOM	1520	CB	GLN	193	15.265	25.621	99.842	1.00	20.00
ATOM	1521	CG	GLN	193	15.034	26.442	98.571	1.00	20.00
ATOM	1522	CD	GLN	193	13.564	26.787	98.487	1.00	20.00
ATOM	1523	OE1	GLN	193	12.685	25.942	98.699	1.00	20.00
ATOM	1524	NE2	GLN	193	13.257	28.078	98.180	1.00	20.00
ATOM	1525	C	GLN	193	17.226	26.890	100.449	1.00	20.00
ATOM	1526	O	GLN	193	17.903	27.478	99.607	1.00	20.00
ATOM	1527	N	GLN	194	16.865	27.457	101.611	1.00	20.00
ATOM	1528	CA	GLN	194	17.176	28.820	101.927	1.00	20.00
ATOM	1529	CB	GLN	194	16.434	29.341	103.168	1.00	20.00
ATOM	1530	CG	GLN	194	14.946	29.591	102.911	1.00	20.00
ATOM	1531	CD	GLN	194	14.829	30.818	102.012	1.00	20.00
ATOM	1532	OE1	GLN	194	14.266	31.837	102.409	1.00	20.00
ATOM	1533	NE2	GLN	194	15.375	30.727	100.770	1.00	20.00
ATOM	1534	C	GLN	194	18.636	29.041	102.144	1.00	20.00
ATOM	1535	O	GLN	194	19.155	30.084	101.751	1.00	20.00
ATOM	1536	N	CYS	195	19.338	28.079	102.772	1.00	20.00
ATOM	1537	CA	CYS	195	20.717	28.305	103.100	1.00	20.00
ATOM	1538	CB	CYS	195	21.440	27.122	103.762	1.00	20.00
ATOM	1539	SG	CYS	195	20.920	26.836	105.478	1.00	20.00
ATOM	1540	C	CYS	195	21.489	28.676	101.881	1.00	20.00

Figure 6 (continued)

ATOM	1541	O	CYS	195	21.258	28.163	100.786	1.00	20.00
ATOM	1542	N	SER	196	22.420	29.630	102.061	1.00	20.00
ATOM	1543	CA	SER	196	23.256	30.065	100.995	1.00	20.00
ATOM	1544	CB	SER	196	23.147	31.578	100.711	1.00	20.00
ATOM	1545	OG	SER	196	24.007	31.930	99.640	1.00	20.00
ATOM	1546	C	SER	196	24.654	29.809	101.435	1.00	20.00
ATOM	1547	O	SER	196	24.961	29.857	102.626	1.00	20.00
ATOM	1548	N	GLY	197	25.546	29.508	100.476	1.00	20.00
ATOM	1549	CA	GLY	197	26.896	29.237	100.853	1.00	20.00
ATOM	1550	C	GLY	197	26.969	27.802	101.256	1.00	20.00
ATOM	1551	O	GLY	197	26.984	26.911	100.404	1.00	20.00
ATOM	1552	N	ARG	198	27.018	27.536	102.578	1.00	20.00
ATOM	1553	CA	ARG	198	27.135	26.178	103.026	1.00	20.00
ATOM	1554	CB	ARG	198	28.563	25.809	103.458	1.00	20.00
ATOM	1555	CG	ARG	198	29.628	26.165	102.416	1.00	20.00
ATOM	1556	CD	ARG	198	29.342	25.646	101.005	1.00	20.00
ATOM	1557	NE	ARG	198	30.472	26.087	100.137	1.00	20.00
ATOM	1558	CZ	ARG	198	30.458	27.330	99.573	1.00	20.00
ATOM	1559	NH1	ARG	198	29.415	28.178	99.807	1.00	20.00
ATOM	1560	NH2	ARG	198	31.493	27.730	98.778	1.00	20.00
ATOM	1561	C	ARG	198	26.263	26.027	104.229	1.00	20.00
ATOM	1562	O	ARG	198	25.555	26.956	104.610	1.00	20.00
ATOM	1563	N	CYS	199	26.261	24.821	104.836	1.00	20.00
ATOM	1564	CA	CYS	199	25.438	24.635	105.994	1.00	20.00
ATOM	1565	CB	CYS	199	24.029	24.136	105.630	1.00	20.00
ATOM	1566	SG	CYS	199	24.083	22.554	104.740	1.00	20.00
ATOM	1567	C	CYS	199	26.071	23.617	106.894	1.00	20.00
ATOM	1568	O	CYS	199	26.749	22.697	106.437	1.00	20.00
ATOM	1569	N	ARG	200	25.879	23.765	108.220	1.00	20.00
ATOM	1570	CA	ARG	200	26.388	22.864	109.176	1.00	20.00
ATOM	1571	CB	ARG	200	26.172	23.288	110.631	1.00	20.00
ATOM	1572	CG	ARG	200	26.619	22.240	111.653	1.00	20.00
ATOM	1573	CD	ARG	200	26.231	22.582	113.092	1.00	20.00
ATOM	1574	NE	ARG	200	26.636	21.432	113.950	1.00	20.00
ATOM	1575	CZ	ARG	200	25.759	20.411	114.180	1.00	20.00
ATOM	1576	NH1	ARG	200	24.507	20.448	113.637	1.00	20.00
ATOM	1577	NH2	ARG	200	26.138	19.352	114.953	1.00	20.00
ATOM	1578	C	ARG	200	25.634	21.573	108.991	1.00	20.00
ATOM	1579	O	ARG	200	26.211	20.486	108.928	1.00	20.00
ATOM	1580	N	GLY	201	24.300	21.689	108.878	1.00	20.00
ATOM	1581	CA	GLY	201	23.466	20.541	108.701	1.00	20.00
ATOM	1582	C	GLY	201	22.804	20.899	107.422	1.00	20.00
ATOM	1583	O	GLY	201	22.487	22.032	107.146	1.00	20.00
ATOM	1584	N	LYS	202	21.671	19.931	107.205	1.00	20.00
ATOM	1585	CA	LYS	202	20.746	20.212	106.151	1.00	20.00
ATOM	1586	CB	LYS	202	19.964	18.978	105.669	1.00	20.00
ATOM	1587	CG	LYS	202	18.904	18.489	106.655	1.00	20.00
ATOM	1588	CD	LYS	202	17.921	17.492	106.037	1.00	20.00
ATOM	1589	CE	LYS	202	16.722	17.176	106.953	1.00	20.00
ATOM	1590	NZ	LYS	202	17.175	16.521	108.180	1.00	20.00
ATOM	1591	C	LYS	202	19.757	21.209	106.664	1.00	20.00
ATOM	1592	O	LYS	202	19.178	21.971	105.893	1.00	20.00
ATOM	1593	N	SER	203	19.547	21.236	107.993	1.00	20.00
ATOM	1594	CA	SER	203	18.590	22.136	108.566	1.00	20.00
ATOM	1595	CB	SER	203	18.554	22.101	110.103	1.00	20.00
ATOM	1596	OG	SER	203	19.783	22.579	110.629	1.00	20.00
ATOM	1597	C	SER	203	18.935	23.531	108.156	1.00	20.00
ATOM	1598	O	SER	203	20.099	23.904	108.017	1.00	20.00
ATOM	1599	N	PRO	204	17.900	24.290	107.926	1.00	20.00
ATOM	1600	CA	PRO	204	18.059	25.667	107.545	1.00	20.00
ATOM	1601	CD	PRO	204	16.689	23.710	107.368	1.00	20.00
ATOM	1602	CB	PRO	204	16.707	26.108	106.989	1.00	20.00
ATOM	1603	CG	PRO	204	16.076	24.803	106.477	1.00	20.00
ATOM	1604	C	PRO	204	18.513	26.498	108.699	1.00	20.00
ATOM	1605	O	PRO	204	18.963	27.622	108.484	1.00	20.00
ATOM	1606	N	SER	205	18.384	25.979	109.931	1.00	20.00
ATOM	1607	CA	SER	205	18.742	26.753	111.079	1.00	20.00
ATOM	1608	CB	SER	205	18.444	26.033	112.403	1.00	20.00
ATOM	1609	OG	SER	205	18.925	26.855	113.496	1.00	20.00
ATOM	1610	C	SER	205	20.208	27.037	111.052	1.00	20.00
ATOM	1611	O	SER	205	20.633	28.159	111.324	1.00	20.00
ATOM	1612	N	ASP	206	21.029	26.027	110.714	1.00	20.00
ATOM	1613	CA	ASP	206	22.436	26.268	110.780	1.00	20.00
ATOM	1614	CB	ASP	206	23.208	25.157	111.522	1.00	20.00
ATOM	1615	CG	ASP	206	22.967	23.823	110.833	1.00	20.00
ATOM	1616	OD1	ASP	206	22.185	23.798	109.844	1.00	20.00
ATOM	1617	OD2	ASP	206	23.553	22.807	111.293	1.00	20.00

Figure 6 (continued)

ATOM	1618	C	ASP	206	23.009	26.457	109.416	1.00 20.00
ATOM	1619	O	ASP	206	23.739	25.610	108.904	1.00 20.00
ATOM	1620	N	CYS	207	22.698	27.600	106.781	1.00 20.00
ATOM	1621	CA	CYS	207	23.320	27.850	107.520	1.00 20.00
ATOM	1622	CB	CYS	207	22.685	28.994	106.712	1.00 20.00
ATOM	1623	SG	CYS	207	20.941	28.696	106.295	1.00 20.00
ATOM	1624	C	CYS	207	24.714	28.257	107.862	1.00 20.00
ATOM	1625	O	CYS	207	25.069	28.244	109.060	1.00 20.00
ATOM	1626	N	CYS	208	25.558	28.599	106.851	1.00 20.00
ATOM	1627	CA	CYS	208	26.904	28.962	107.257	1.00 20.00
ATOM	1628	CB	CYS	208	28.002	28.034	106.684	1.00 20.00
ATOM	1629	SG	CYS	208	27.933	26.297	107.211	1.00 20.00
ATOM	1630	C	CYS	208	27.192	30.318	106.673	1.00 20.00
ATOM	1631	O	CYS	208	28.354	30.904	105.978	1.00 20.00
ATOM	1632	N	HIS	209	26.378	30.856	106.983	1.00 20.00
ATOM	1633	CA	HIS	209	26.761	32.157	106.516	1.00 20.00
ATOM	1634	ND1	HIS	209	31.205	34.449	105.754	1.00 20.00
ATOM	1635	NE2	HIS	209	30.583	36.333	106.757	1.00 20.00
ATOM	1636	CE1	HIS	209	31.279	35.802	105.767	1.00 20.00
ATOM	1637	CD2	HIS	209	30.033	35.247	107.414	1.00 20.00
ATOM	1638	CG	HIS	209	30.404	34.084	106.813	1.00 20.00
ATOM	1639	CB	HIS	209	30.067	32.664	107.158	1.00 20.00
ATOM	1640	C	HIS	209	28.949	32.079	105.033	1.00 20.00
ATOM	1641	O	HIS	209	29.128	31.004	104.466	1.00 20.00
ATOM	1642	N	ASN	210	28.893	33.246	104.387	1.00 20.00
ATOM	1643	CA	ASN	210	29.004	33.331	102.939	1.00 20.00
ATOM	1644	CB	ASN	210	28.846	34.774	102.478	1.00 20.00
ATOM	1645	CG	ASN	210	28.714	34.761	100.911	1.00 20.00
ATOM	1646	OD1	ASN	210	28.082	33.733	100.258	1.00 20.00
ATOM	1647	ND2	ASN	210	28.416	35.952	100.326	1.00 20.00
ATOM	1648	C	ASN	210	30.363	32.852	102.527	1.00 20.00
ATOM	1649	O	ASN	210	30.515	32.222	101.481	1.00 20.00
ATOM	1650	N	GLN	211	31.390	33.178	103.333	1.00 20.00
ATOM	1651	CA	GLN	211	32.767	32.859	103.063	1.00 20.00
ATOM	1652	CB	GLN	211	33.737	33.596	104.003	1.00 20.00
ATOM	1653	CG	GLN	211	33.714	35.117	103.836	1.00 20.00
ATOM	1654	CD	GLN	211	34.323	35.463	102.486	1.00 20.00
ATOM	1655	OE1	GLN	211	34.693	34.585	101.701	1.00 20.00
ATOM	1656	NE2	GLN	211	34.447	36.787	102.201	1.00 20.00
ATOM	1657	C	GLN	211	33.052	31.398	103.194	1.00 20.00
ATOM	1658	O	GLN	211	33.949	30.857	102.430	1.00 20.00
ATOM	1659	N	CYS	212	32.426	30.716	104.172	1.00 20.00
ATOM	1660	CA	CYS	212	32.752	29.336	104.389	1.00 20.00
ATOM	1661	CB	CYS	212	31.903	28.637	105.463	1.00 20.00
ATOM	1662	SG	CYS	212	32.242	29.235	107.138	1.00 20.00
ATOM	1663	C	CYS	212	32.532	28.570	103.132	1.00 20.00
ATOM	1664	O	CYS	212	31.684	28.890	102.334	1.00 20.00
ATOM	1665	N	ALA	213	33.386	27.555	102.909	1.00 20.00
ATOM	1666	CA	ALA	213	33.223	26.691	101.786	1.00 20.00
ATOM	1667	CB	ALA	213	34.360	26.783	100.754	1.00 20.00
ATOM	1668	C	ALA	213	33.221	25.317	102.367	1.00 20.00
ATOM	1669	O	ALA	213	33.860	25.080	103.391	1.00 20.00
ATOM	1670	N	ALA	214	32.475	24.386	101.743	1.00 20.00
ATOM	1671	CA	ALA	214	32.371	23.039	102.226	1.00 20.00
ATOM	1672	CB	ALA	214	33.677	22.431	102.779	1.00 20.00
ATOM	1673	C	ALA	214	31.310	22.983	103.291	1.00 20.00
ATOM	1674	O	ALA	214	30.179	22.609	103.012	1.00 20.00
ATOM	1675	N	GLY	215	31.668	23.351	104.545	1.00 20.00
ATOM	1676	CA	GLY	215	30.697	23.270	105.605	1.00 20.00
ATOM	1677	C	GLY	215	31.138	24.140	106.743	1.00 20.00
ATOM	1678	O	GLY	215	31.970	25.030	106.574	1.00 20.00
ATOM	1679	N	CYS	216	30.546	23.934	107.939	1.00 20.00
ATOM	1680	CA	CYS	216	30.951	24.718	109.070	1.00 20.00
ATOM	1681	CB	CYS	216	30.396	26.163	109.060	1.00 20.00
ATOM	1682	SG	CYS	216	28.581	26.299	109.142	1.00 20.00
ATOM	1683	C	CYS	216	30.505	24.039	110.327	1.00 20.00
ATOM	1684	O	CYS	216	29.540	23.275	110.333	1.00 20.00
ATOM	1685	N	THR	217	31.244	24.267	111.432	1.00 20.00
ATOM	1686	CA	THR	217	30.866	23.699	112.693	1.00 20.00
ATOM	1687	CB	THR	217	31.891	23.910	113.766	1.00 20.00
ATOM	1688	OG1	THR	217	32.063	25.297	114.016	1.00 20.00
ATOM	1689	CG2	THR	217	33.215	23.275	113.306	1.00 20.00
ATOM	1690	C	THR	217	29.606	24.371	113.122	1.00 20.00
ATOM	1691	O	THR	217	28.677	23.731	113.613	1.00 20.00
ATOM	1692	N	GLY	218	29.556	25.702	112.929	1.00 20.00
ATOM	1693	CA	GLY	218	28.405	26.480	113.274	1.00 20.00
ATOM	1694	C	GLY	218	28.579	27.771	132.553	1.00 20.00

Figure 6 (continued)

ATOM	1695	O	GLY	218	29.687	28.095	112.124	1.00	20.00
ATOM	1696	N	PRO	219	27.507	28.500	112.390	1.00	20.00
ATOM	1697	CA	PRO	219	27.565	29.761	111.672	1.00	20.00
ATOM	1698	CD	PRO	219	26.471	28.480	113.348	1.00	20.00
ATOM	1699	CB	PRO	219	26.186	30.370	111.845	1.00	20.00
ATOM	1700	CG	PRO	219	26.757	29.869	113.237	1.00	20.00
ATOM	1701	C	PRO	219	28.636	30.604	112.263	1.00	20.00
ATOM	1702	O	PRO	219	28.406	31.211	113.307	1.00	20.00
ATOM	1703	N	ARG	220	29.802	30.688	111.593	1.00	20.00
ATOM	1704	CA	ARG	220	30.887	31.495	112.065	1.00	20.00
ATOM	1705	CB	ARG	220	31.665	30.870	113.235	1.00	20.00
ATOM	1706	CG	ARG	220	30.825	30.632	114.489	1.00	20.00
ATOM	1707	CD	ARG	220	30.773	31.832	115.432	1.00	20.00
ATOM	1708	NE	ARG	220	30.158	32.053	116.935	1.00	20.00
ATOM	1709	CZ	ARG	220	32.483	33.227	116.550	1.00	20.00
ATOM	1710	NH1	ARG	220	31.532	34.190	116.720	1.00	20.00
ATOM	1711	NH2	ARG	220	33.755	33.453	116.990	1.00	20.00
ATOM	1712	C	ARG	220	31.867	31.565	110.941	1.00	20.00
ATOM	1713	O	ARG	220	31.987	30.628	110.154	1.00	20.00
ATOM	1714	N	GLU	221	32.594	32.690	110.835	1.00	20.00
ATOM	1715	CA	GLU	221	33.599	32.859	109.825	1.00	20.00
ATOM	1716	CB	GLU	221	34.140	34.288	109.775	1.00	20.00
ATOM	1717	CG	GLU	221	33.069	35.307	109.379	1.00	20.00
ATOM	1718	CD	GLU	221	33.694	36.692	109.420	1.00	20.00
ATOM	1719	OE1	GLU	221	34.946	36.771	109.530	1.00	20.00
ATOM	1720	OE2	GLU	221	32.998	37.691	109.343	1.00	20.00
ATOM	1721	C	GLU	221	34.739	31.934	110.156	1.00	20.00
ATOM	1722	O	GLU	221	35.399	31.392	109.271	1.00	20.00
ATOM	1723	N	SER	222	35.024	31.785	111.462	1.00	20.00
ATOM	1724	CA	SER	222	36.091	30.965	111.970	1.00	20.00
ATOM	1725	CB	SER	222	36.398	31.242	113.453	1.00	20.00
ATOM	1726	OG	SER	222	35.300	30.868	114.261	1.00	20.00
ATOM	1727	C	SER	222	35.754	29.507	111.851	1.00	20.00
ATOM	1728	O	SER	222	36.642	28.664	111.741	1.00	20.00
ATOM	1729	N	ASP	223	34.451	29.179	111.904	1.00	20.00
ATOM	1730	CA	ASP	223	33.949	27.831	111.941	1.00	20.00
ATOM	1731	CB	ASP	223	32.461	27.745	112.315	1.00	20.00
ATOM	1732	CG	ASP	223	32.362	28.062	113.802	1.00	20.00
ATOM	1733	OD1	ASP	223	33.407	28.447	114.393	1.00	20.00
ATOM	1734	OD2	ASP	223	31.247	27.918	114.371	1.00	20.00
ATOM	1735	C	ASP	223	34.169	27.068	110.685	1.00	20.00
ATOM	1736	O	ASP	223	34.130	25.839	110.685	1.00	20.00
ATOM	1737	N	CYS	224	34.339	27.764	109.527	1.00	20.00
ATOM	1738	CA	CYS	224	34.448	27.151	108.225	1.00	20.00
ATOM	1739	CB	CYS	224	35.043	28.080	107.159	1.00	20.00
ATOM	1740	SG	CYS	224	34.212	29.696	107.044	1.00	20.00
ATOM	1741	C	CYS	224	35.353	25.951	108.244	1.00	20.00
ATOM	1742	O	CYS	224	36.306	25.875	109.018	1.00	20.00
ATOM	1743	N	LEU	225	34.984	24.921	107.449	1.00	20.00
ATOM	1744	CA	LEU	225	35.807	23.766	107.222	1.00	20.00
ATOM	1745	CB	LEU	225	34.996	22.552	106.727	1.00	20.00
ATOM	1746	CG	LEU	225	33.995	22.038	107.776	1.00	20.00
ATOM	1747	CD1	LEU	225	33.262	20.781	107.283	1.00	20.00
ATOM	1748	CD2	LEU	225	34.668	21.843	109.145	1.00	20.00
ATOM	1749	C	LEU	225	36.828	24.117	106.185	1.00	20.00
ATOM	1750	O	LEU	225	37.931	23.578	106.177	1.00	20.00
ATOM	1751	N	VAL	226	36.443	25.009	105.246	1.00	20.00
ATOM	1752	CA	VAL	226	37.293	25.435	104.173	1.00	20.00
ATOM	1753	CB	VAL	226	37.158	24.548	102.967	1.00	20.00
ATOM	1754	CG1	VAL	226	38.085	25.028	101.837	1.00	20.00
ATOM	1755	CG2	VAL	226	37.438	23.100	103.414	1.00	20.00
ATOM	1756	C	VAL	226	36.854	26.821	103.807	1.00	20.00
ATOM	1757	O	VAL	226	35.787	27.264	104.225	1.00	20.00
ATOM	1758	N	CYS	227	37.669	27.551	103.012	1.00	20.00
ATOM	1759	CA	CYS	227	37.333	28.910	102.701	1.00	20.00
ATOM	1760	CB	CYS	227	38.489	29.866	103.045	1.00	20.00
ATOM	1761	SG	CYS	227	38.093	31.630	102.904	1.00	20.00
ATOM	1762	C	CYS	227	37.019	29.003	101.239	1.00	20.00
ATOM	1763	O	CYS	227	37.584	28.279	100.420	1.00	20.00
ATOM	1764	N	ARG	228	36.044	29.869	100.888	1.00	20.00
ATOM	1765	CA	ARG	228	35.667	30.087	99.520	1.00	20.00
ATOM	1766	CB	ARG	228	34.418	30.945	99.346	1.00	20.00
ATOM	1767	CG	ARG	228	34.001	31.131	97.874	1.00	20.00
ATOM	1768	CD	ARG	228	32.728	31.856	97.637	1.00	20.00
ATOM	1769	NE	ARG	228	32.565	31.975	96.161	1.00	20.00
ATOM	1770	CZ	ARG	228	32.078	30.924	95.439	1.00	20.00
ATOM	1771	NH1	ARG	228	31.740	29.762	96.070	1.00	20.00

Figure 6 (continued)

ATOM	1772	NH2	ARG	228	31.935	31.036	94.086	1.00 20.00
ATOM	1773	C	ARG	228	36.790	30.753	98.823	1.00 20.00
ATOM	1774	O	ARG	228	37.171	30.369	97.710	1.00 20.00
ATOM	1775	N	LYS	229	37.366	31.763	99.496	1.00 20.00
ATOM	1776	CA	LYS	229	38.413	32.542	98.910	1.00 20.00
ATOM	1777	CB	LYS	229	38.191	34.057	99.044	1.00 20.00
ATOM	1778	CG	LYS	229	37.042	34.561	98.171	1.00 20.00
ATOM	1779	CD	LYS	229	37.253	34.283	96.680	1.00 20.00
ATOM	1780	CE	LYS	229	36.105	34.761	95.790	1.00 20.00
ATOM	1781	NZ	LYS	229	36.184	36.227	95.603	1.00 20.00
ATOM	1782	C	LYS	229	39.687	32.194	99.601	1.00 20.00
ATOM	1783	O	LYS	229	40.193	31.078	99.477	1.00 20.00
ATOM	1784	N	PHE	230	40.258	33.164	100.336	1.00 20.00
ATOM	1785	CA	PHE	230	41.529	32.907	100.942	1.00 20.00
ATOM	1786	CB	PHE	230	42.569	33.977	100.583	1.00 20.00
ATOM	1787	CG	PHE	230	42.657	33.954	99.093	1.00 20.00
ATOM	1788	CD1	PHE	230	43.536	33.115	98.450	1.00 20.00
ATOM	1789	CD2	PHE	230	41.839	34.761	98.336	1.00 20.00
ATOM	1790	CE1	PHE	230	43.610	33.092	97.077	1.00 20.00
ATOM	1791	CE2	PHE	230	41.908	34.743	96.963	1.00 20.00
ATOM	1792	CZ	PHE	230	42.793	33.906	96.330	1.00 20.00
ATOM	1793	C	PHE	230	41.368	32.874	102.427	1.00 20.00
ATOM	1794	O	PHE	230	40.583	33.627	102.998	1.00 20.00
ATOM	1795	N	ARG	231	42.120	31.974	103.091	1.00 20.00
ATOM	1796	CA	ARG	231	42.039	31.849	104.516	1.00 20.00
ATOM	1797	CB	ARG	231	42.237	30.409	105.019	1.00 20.00
ATOM	1798	CG	ARG	231	41.072	29.470	104.701	1.00 20.00
ATOM	1799	CD	ARG	231	40.210	29.136	105.921	1.00 20.00
ATOM	1800	NE	ARG	231	41.072	28.375	106.870	1.00 20.00
ATOM	1801	CZ	ARG	231	40.647	28.124	108.142	1.00 20.00
ATOM	1802	NH1	ARG	231	39.422	28.566	108.553	1.00 20.00
ATOM	1803	NH2	ARG	231	41.447	27.430	109.002	1.00 20.00
ATOM	1804	C	ARG	231	43.141	32.670	105.095	1.00 20.00
ATOM	1805	O	ARG	231	44.256	32.668	104.574	1.00 20.00
ATOM	1806	N	ASP	232	42.846	33.433	106.148	1.00 20.00
ATOM	1807	CA	ASP	232	43.808	34.220	106.741	1.00 20.00
ATOM	1808	CB	ASP	232	43.974	35.641	106.150	1.00 20.00
ATOM	1809	CG	ASP	232	45.245	36.315	106.653	1.00 20.00
ATOM	1810	OD1	ASP	232	45.995	35.669	107.431	1.00 20.00
ATOM	1811	OD2	ASP	232	45.485	37.488	106.260	1.00 20.00
ATOM	1812	C	ASP	232	43.611	34.358	108.202	1.00 20.00
ATOM	1813	O	ASP	232	42.499	34.684	108.606	1.00 20.00
ATOM	1814	N	GLU	233	44.636	34.109	109.035	1.00 20.00
ATOM	1815	CA	GLU	233	44.517	34.286	110.453	1.00 20.00
ATOM	1816	CB	GLU	233	44.360	35.763	110.853	1.00 20.00
ATOM	1817	CG	GLU	233	45.572	36.628	110.505	1.00 20.00
ATOM	1818	CD	GLU	233	45.258	38.056	110.930	1.00 20.00
ATOM	1819	OE1	GLU	233	45.031	38.275	112.150	1.00 20.00
ATOM	1820	OE2	GLU	233	45.235	38.967	110.040	1.00 20.00
ATOM	1821	C	GLU	233	43.320	33.557	110.969	1.00 20.00
ATOM	1822	O	GLU	233	42.500	34.129	111.685	1.00 20.00
ATOM	1823	N	ALA	234	43.190	32.266	110.622	1.00 20.00
ATOM	1824	CA	ALA	234	42.116	31.473	111.146	1.00 20.00
ATOM	1825	CB	ALA	234	42.111	31.424	112.683	1.00 20.00
ATOM	1826	C	ALA	234	40.796	32.011	110.689	1.00 20.00
ATOM	1827	O	ALA	234	39.753	31.543	111.143	1.00 20.00
ATOM	1828	N	THR	235	40.781	32.995	109.769	1.00 20.00
ATOM	1829	CA	THR	235	39.503	33.482	109.337	1.00 20.00
ATOM	1830	CB	THR	235	39.288	34.931	109.648	1.00 20.00
ATOM	1831	OG1	THR	235	40.180	35.753	108.951	1.00 20.00
ATOM	1832	CG2	THR	235	39.406	35.140	111.163	1.00 20.00
ATOM	1833	C	THR	235	39.416	33.319	107.855	1.00 20.00
ATOM	1834	O	THR	235	40.417	33.394	107.146	1.00 20.00
ATOM	1835	N	CYS	236	38.192	33.078	107.349	1.00 20.00
ATOM	1836	CA	CYS	236	38.001	32.892	105.947	1.00 20.00
ATOM	1837	CB	CYS	236	36.800	31.972	105.650	1.00 20.00
ATOM	1838	SG	CYS	236	36.337	31.820	103.901	1.00 20.00
ATOM	1839	C	CYS	236	37.757	34.243	105.357	1.00 20.00
ATOM	1840	O	CYS	236	36.743	34.876	105.644	1.00 20.00
ATOM	1841	N	LYS	237	38.699	34.721	104.515	1.00 20.00
ATOM	1842	CA	LYS	237	38.564	36.042	103.976	1.00 20.00
ATOM	1843	CB	LYS	237	39.768	36.950	104.271	1.00 20.00
ATOM	1844	CG	LYS	237	39.902	37.225	105.768	1.00 20.00
ATOM	1845	CD	LYS	237	38.629	37.821	106.374	1.00 20.00
ATOM	1846	CE	LYS	237	38.625	37.859	107.902	1.00 20.00
ATOM	1847	NZ	LYS	237	37.326	38.377	108.387	1.00 20.00
ATOM	1848	C	LYS	237	38.358	35.977	102.495	1.00 20.00

Figure 6 (continued)

ATOM	1845	O	LYS	237	38.846	35.079	101.814	1.00	20.00
ATOM	1850	N	ASP	238	37.555	36.936	101.986	1.00	20.00
ATOM	1851	CA	ASP	238	37.223	37.680	100.596	1.00	20.00
ATOM	1852	CB	ASP	238	36.171	36.185	100.390	1.00	20.00
ATOM	1853	CG	ASP	238	35.744	36.227	98.928	1.00	20.00
ATOM	1854	OD1	ASP	238	36.331	37.472	98.109	1.00	20.00
ATOM	1855	OD2	ASP	238	34.818	39.023	98.613	1.00	20.00
ATOM	1856	C	ASP	238	38.458	37.477	99.851	1.00	20.00
ATOM	1857	O	ASP	238	38.737	36.982	98.760	1.00	20.00
ATOM	1858	N	THR	239	39.224	38.411	100.431	1.00	20.00
ATOM	1859	CA	THR	239	40.448	38.854	99.832	1.00	20.00
ATOM	1860	CB	THR	239	40.329	40.155	99.097	1.00	20.00
ATOM	1861	OG1	THR	239	39.549	41.189	99.993	1.00	20.00
ATOM	1862	CG2	THR	239	39.977	39.958	97.987	1.00	20.00
ATOM	1863	C	THR	239	41.365	39.080	100.978	1.00	20.00
ATOM	1864	O	THR	239	40.916	39.209	102.116	1.00	20.00
ATOM	1865	N	CYS	240	42.683	39.120	100.733	1.00	20.00
ATOM	1866	CA	CYS	240	43.501	39.293	101.887	1.00	20.00
ATOM	1867	CB	CYS	240	44.812	38.515	101.839	1.00	20.00
ATOM	1868	SG	CYS	240	44.408	36.753	101.902	1.00	20.00
ATOM	1869	C	CYS	240	43.713	40.740	102.138	1.00	20.00
ATOM	1870	O	CYS	240	43.757	41.576	101.237	1.00	20.00
ATOM	1871	N	PRO	241	43.721	41.043	103.407	1.00	60.00
ATOM	1872	CA	PRO	241	44.007	42.383	103.837	1.00	60.00
ATOM	1873	CD	PRO	241	42.818	40.363	104.319	1.00	60.00
ATOM	1874	CB	PRO	241	43.277	42.577	105.167	1.00	60.00
ATOM	1875	CG	PRO	241	42.933	41.151	105.631	1.00	60.00
ATOM	1876	C	PRO	241	45.485	42.554	103.951	1.00	60.00
ATOM	1877	O	PRO	241	46.175	41.569	104.269	1.00	60.00
ATOM	1878	N	PRO	242	45.980	43.743	103.769	1.00	60.00
ATOM	1879	CA	PRO	242	47.389	43.977	103.902	1.00	60.00
ATOM	1880	CD	PRO	242	45.202	44.947	104.007	1.00	60.00
ATOM	1881	CB	PRO	242	47.555	45.407	103.767	1.00	60.00
ATOM	1882	CG	PRO	242	46.240	46.028	104.359	1.00	60.00
ATOM	1883	C	PRO	242	47.770	43.533	105.276	1.00	60.00
ATOM	1884	O	PRO	242	48.805	43.053	105.471	1.00	60.00
ATOM	1885	N	LEU	243	46.880	43.712	106.240	1.00	60.00
ATOM	1886	CA	LEU	243	47.089	43.368	107.608	1.00	60.00
ATOM	1887	CB	LEU	243	47.709	44.505	108.438	1.00	60.00
ATOM	1888	CG	LEU	243	49.158	44.819	108.040	1.00	60.00
ATOM	1889	CD1	LEU	243	49.746	45.960	108.883	1.00	60.00
ATOM	1890	CD2	LEU	243	50.013	43.547	108.079	1.00	60.00
ATOM	1891	C	LEU	243	45.751	43.091	108.189	1.00	60.00
ATOM	1892	O	LEU	243	44.871	42.571	107.504	1.00	60.00
ATOM	1893	N	MET	244	45.582	43.414	109.486	1.00	60.00
ATOM	1894	CA	MET	244	44.310	43.219	110.108	1.00	60.00
ATOM	1895	CB	MET	244	44.244	43.768	111.544	1.00	60.00
ATOM	1896	CG	MET	244	44.404	45.269	111.623	1.00	60.00
ATOM	1897	SD	MET	244	46.031	45.916	111.113	1.00	60.00
ATOM	1898	CE	MET	244	45.606	47.607	111.417	1.00	60.00
ATOM	1899	C	MET	244	43.341	43.983	109.277	1.00	60.00
ATOM	1900	O	MET	244	43.618	45.108	108.861	1.00	60.00
ATOM	1901	N	LEU	245	42.178	43.377	108.983	1.00	60.00
ATOM	1902	CA	LEU	245	41.275	44.062	108.114	1.00	60.00
ATOM	1903	CB	LEU	245	40.482	43.129	107.184	1.00	60.00
ATOM	1904	CG	LEU	245	39.510	43.877	106.252	1.00	60.00
ATOM	1905	CD1	LEU	245	40.262	44.818	105.295	1.00	60.00
ATOM	1906	CD2	LEU	245	38.586	42.898	105.511	1.00	60.00
ATOM	1907	C	LEU	245	40.300	44.820	108.945	1.00	60.00
ATOM	1908	O	LEU	245	39.603	44.260	109.791	1.00	60.00
ATOM	1909	N	TYR	246	40.255	46.143	108.713	1.00	60.00
ATOM	1910	CA	TYR	246	39.356	47.021	109.391	1.00	60.00
ATOM	1911	CB	TYR	246	39.974	47.732	110.606	1.00	60.00
ATOM	1912	CG	TYR	246	40.210	46.669	111.624	1.00	60.00
ATOM	1913	CD1	TYR	246	39.183	46.232	112.429	1.00	60.00
ATOM	1914	CD2	TYR	246	41.454	46.100	111.770	1.00	60.00
ATOM	1915	CE1	TYR	246	39.392	45.248	113.367	1.00	60.00
ATOM	1916	CE2	TYR	246	41.669	45.115	112.706	1.00	60.00
ATOM	1917	CZ	TYR	246	40.638	44.686	113.506	1.00	60.00
ATOM	1918	OH	TYR	246	40.858	43.675	114.466	1.00	60.00
ATOM	1919	C	TYR	246	38.956	48.037	108.378	1.00	60.00
ATOM	1920	O	TYR	246	39.319	47.918	107.209	1.00	60.00
ATOM	1921	N	ASN	247	38.163	49.044	108.784	1.00	60.00
ATOM	1922	CA	ASN	247	37.735	50.024	107.830	1.00	60.00
ATOM	1923	CB	ASN	247	36.209	50.469	108.073	1.00	60.00
ATOM	1924	CG	ASN	247	35.918	51.523	107.024	1.00	60.00
ATOM	1925	OD1	ASN	247	36.117	52.719	107.228	1.00	60.00

Figure 6 (continued)

ATOM	1926	ND2	ASN	247	35.367	51.057	105.671	1.00	60.00
ATOM	1927	C	ASN	247	38.635	51.213	107.946	1.00	60.00
ATOM	1928	O	ASN	247	38.717	51.854	108.992	1.00	60.00
ATOM	1929	N	PRO	248	39.339	51.502	106.887	1.00	60.00
ATOM	1930	CA	PRO	248	40.192	52.656	106.911	1.00	60.00
ATOM	1931	CD	PRO	248	39.911	50.433	106.084	1.00	60.00
ATOM	1932	CB	PRO	248	41.218	52.451	105.801	1.00	60.00
ATOM	1933	CG	PRO	248	41.306	50.922	105.667	1.00	60.00
ATOM	1934	C	PRO	248	39.351	53.868	106.711	1.00	60.00
ATOM	1935	O	PRO	248	38.223	53.733	106.242	1.00	60.00
ATOM	1936	N	THR	249	39.871	55.061	107.053	1.00	60.00
ATOM	1937	CA	THR	249	39.086	56.239	106.847	1.00	60.00
ATOM	1938	CB	THR	249	39.776	57.502	107.296	1.00	60.00
ATOM	1939	OG1	THR	249	38.891	58.607	107.183	1.00	60.00
ATOM	1940	CG2	THR	249	41.042	57.740	106.455	1.00	60.00
ATOM	1941	C	THR	249	38.823	56.315	105.381	1.00	60.00
ATOM	1942	O	THR	249	37.710	56.613	104.951	1.00	60.00
ATOM	1943	N	THR	250	39.852	56.015	104.568	1.00	60.00
ATOM	1944	CA	THR	250	39.673	56.034	103.151	1.00	60.00
ATOM	1945	CB	THR	250	40.961	56.078	102.379	1.00	60.00
ATOM	1946	OG1	THR	250	40.698	56.296	101.001	1.00	60.00
ATOM	1947	CG2	THR	250	41.708	54.748	102.575	1.00	60.00
ATOM	1948	C	THR	250	38.962	54.774	102.789	1.00	60.00
ATOM	1949	O	THR	250	38.895	53.835	103.582	1.00	60.00
ATOM	1950	N	TYR	251	38.386	54.732	101.575	1.00	60.00
ATOM	1951	CA	TYR	251	37.687	53.553	101.168	1.00	60.00
ATOM	1952	CB	TYR	251	36.806	53.729	99.916	1.00	60.00
ATOM	1953	CG	TYR	251	35.559	54.427	100.344	1.00	60.00
ATOM	1954	CD1	TYR	251	35.513	55.794	100.493	1.00	60.00
ATOM	1955	CD2	TYR	251	34.422	53.694	100.598	1.00	60.00
ATOM	1956	CE1	TYR	251	34.351	56.416	100.892	1.00	60.00
ATOM	1957	CE2	TYR	251	33.260	54.308	100.996	1.00	60.00
ATOM	1958	CZ	TYR	251	33.222	55.673	101.145	1.00	60.00
ATOM	1959	OH	TYR	251	32.028	56.303	101.556	1.00	60.00
ATOM	1960	C	TYR	251	38.680	52.474	100.905	1.00	60.00
ATOM	1961	O	TYR	251	39.886	52.711	100.849	1.00	60.00
ATOM	1962	N	GLN	252	38.166	51.240	100.763	1.00	60.00
ATOM	1963	CA	GLN	252	38.975	50.082	100.535	1.00	60.00
ATOM	1964	CB	GLN	252	38.148	48.790	100.443	1.00	60.00
ATOM	1965	CG	GLN	252	37.505	48.392	101.772	1.00	60.00
ATOM	1966	CD	GLN	252	36.708	47.119	101.544	1.00	60.00
ATOM	1967	OE1	GLN	252	37.174	46.185	100.893	1.00	60.00
ATOM	1968	NE2	GLN	252	35.460	47.086	102.084	1.00	60.00
ATOM	1969	C	GLN	252	39.689	50.261	99.240	1.00	60.00
ATOM	1970	O	GLN	252	40.852	49.882	99.118	1.00	60.00
ATOM	1971	N	MET	253	39.012	50.852	98.238	1.00	60.00
ATOM	1972	CA	MET	253	39.666	51.035	96.978	1.00	60.00
ATOM	1973	CB	MET	253	38.803	51.762	95.932	1.00	60.00
ATOM	1974	CG	MET	253	37.538	50.994	95.541	1.00	60.00
ATOM	1975	SD	MET	253	36.238	50.995	96.811	1.00	60.00
ATOM	1976	CE	MET	253	35.821	52.749	96.594	1.00	60.00
ATOM	1977	C	MET	253	40.861	51.886	97.245	1.00	60.00
ATOM	1978	O	MET	253	40.743	53.069	97.561	1.00	60.00
ATOM	1979	N	ASP	254	42.057	51.277	97.145	1.00	60.00
ATOM	1980	CA	ASP	254	43.266	51.991	97.418	1.00	60.00
ATOM	1981	CB	ASP	254	44.085	51.304	98.570	1.00	60.00
ATOM	1982	CG	ASP	254	43.316	51.402	99.864	1.00	60.00
ATOM	1983	OD1	ASP	254	42.585	52.625	99.951	1.00	60.00
ATOM	1984	OD2	ASP	254	43.444	50.747	100.780	1.00	60.00
ATOM	1985	C	ASP	254	44.116	51.908	96.197	1.00	60.00
ATOM	1986	O	ASP	254	43.918	51.045	95.343	1.00	60.00
ATOM	1987	N	VAL	255	45.089	52.829	96.084	1.00	60.00
ATOM	1988	CA	VAL	255	45.953	52.809	94.946	1.00	60.00
ATOM	1989	CB	VAL	255	46.998	53.885	94.986	1.00	60.00
ATOM	1990	CG1	VAL	255	47.930	53.705	93.775	1.00	60.00
ATOM	1991	CG2	VAL	255	46.297	55.252	95.031	1.00	60.00
ATOM	1992	C	VAL	255	46.667	51.504	94.987	1.00	60.00
ATOM	1993	O	VAL	255	46.804	50.822	93.972	1.00	60.00
ATOM	1994	N	ASN	256	47.126	51.119	96.191	1.00	60.00
ATOM	1995	CA	ASN	256	47.840	49.891	96.350	1.00	60.00
ATOM	1996	CB	ASN	256	48.691	49.839	97.632	1.00	60.00
ATOM	1997	CG	ASN	256	47.769	50.002	98.834	1.00	60.00
ATOM	1998	OD1	ASN	256	47.369	49.029	99.464	1.00	60.00
ATOM	1999	ND2	ASN	256	47.426	51.276	99.160	1.00	60.00
ATOM	2000	C	ASN	256	46.861	48.765	96.388	1.00	60.00
ATOM	2001	O	ASN	256	45.669	48.921	96.648	1.00	60.00
ATOM	2002	N	PRO	257	47.406	47.623	96.086	1.00	60.00

Figure 6 (continued)

ATOM	2003	CA	PRO	257	46.650	46.404	96.101	1.00	60.00
ATOM	2004	CD	PRO	257	48.448	47.551	95.072	1.00	60.00
ATOM	2005	CB	PRO	257	47.457	45.363	96.293	1.00	60.00
ATOM	2006	CG	PRO	257	48.253	46.269	94.314	1.00	60.00
ATOM	2007	C	PRO	257	46.453	46.004	97.521	1.00	60.00
ATOM	2008	O	PRO	257	46.812	46.779	98.406	1.00	60.00
ATOM	2009	N	GLU	258	45.895	44.800	97.748	1.00	60.00
ATOM	2010	CA	GLU	258	45.609	44.329	99.069	1.00	60.00
ATOM	2011	CB	GLU	258	45.214	42.842	99.071	1.00	60.00
ATOM	2012	CG	GLU	258	43.949	42.540	98.261	1.00	60.00
ATOM	2013	CD	GLU	258	42.761	43.181	98.963	1.00	60.00
ATOM	2014	OE1	GLU	258	42.962	43.742	100.073	1.00	60.00
ATOM	2016	OE2	GLU	258	41.637	43.117	98.398	1.00	60.00
ATOM	2016	C	GLU	258	46.878	44.453	99.847	1.00	60.00
ATOM	2017	O	GLU	258	46.881	44.955	100.970	1.00	60.00
ATOM	2018	N	GLY	259	48.003	44.023	99.253	1.00	60.00
ATOM	2019	CA	GLY	259	49.281	44.185	99.918	1.00	60.00
ATOM	2020	C	GLY	259	49.596	42.908	100.603	1.00	60.00
ATOM	2021	O	GLY	259	50.761	42.640	100.895	1.00	60.00
ATOM	2022	N	LYS	260	48.587	42.071	100.880	1.00	60.00
ATOM	2023	CA	LYS	260	48.905	40.825	101.498	1.00	60.00
ATOM	2024	CB	LYS	260	47.732	40.172	102.250	1.00	60.00
ATOM	2025	CG	LYS	260	48.120	38.889	102.989	1.00	60.00
ATOM	2026	CD	LYS	260	49.128	39.111	104.121	1.00	60.00
ATOM	2027	CE	LYS	260	48.621	40.026	105.238	1.00	60.00
ATOM	2028	NZ	LYS	260	47.632	39.310	106.074	1.00	60.00
ATOM	2029	C	LYS	260	49.315	39.934	100.361	1.00	60.00
ATOM	2030	O	LYS	260	49.010	40.209	99.221	1.00	60.00
ATOM	2031	N	TYR	261	50.046	38.847	100.684	1.00	20.00
ATOM	2032	CA	TYR	261	50.449	38.037	99.581	1.00	20.00
ATOM	2033	CB	TYR	261	51.947	37.694	99.596	1.00	20.00
ATOM	2034	CG	TYR	261	52.632	39.011	99.718	1.00	20.00
ATOM	2035	CD1	TYR	261	52.617	39.914	98.681	1.00	20.00
ATOM	2036	CD2	TYR	261	53.241	39.373	100.898	1.00	20.00
ATOM	2037	CE1	TYR	261	53.234	41.137	98.810	1.00	20.00
ATOM	2038	CE2	TYR	261	53.861	40.591	101.025	1.00	20.00
ATOM	2039	CZ	TYR	261	53.863	41.478	99.981	1.00	20.00
ATOM	2040	OH	TYR	261	54.500	42.729	100.118	1.00	20.00
ATOM	2041	C	TYR	261	49.663	36.775	99.661	1.00	20.00
ATOM	2042	O	TYR	261	49.593	36.140	100.712	1.00	20.00
ATOM	2043	N	SER	262	49.030	36.386	98.540	1.00	20.00
ATOM	2044	CA	SER	262	48.241	35.193	98.557	1.00	20.00
ATOM	2045	CB	SER	262	47.000	35.258	97.653	1.00	20.00
ATOM	2046	OG	SER	262	47.396	35.388	96.296	1.00	20.00
ATOM	2047	C	SER	262	49.101	34.091	98.047	1.00	20.00
ATOM	2048	O	SER	262	49.756	34.222	97.014	1.00	20.00
ATOM	2049	N	PHE	263	49.141	32.972	98.791	1.00	20.00
ATOM	2050	CA	PHE	263	49.945	31.874	98.362	1.00	20.00
ATOM	2051	CB	PHE	263	51.182	31.651	99.250	1.00	20.00
ATOM	2052	CG	PHE	263	51.934	30.486	98.706	1.00	20.00
ATOM	2053	CD1	PHE	263	52.842	30.657	97.686	1.00	20.00
ATOM	2054	CD2	PHE	263	51.733	29.224	99.214	1.00	20.00
ATOM	2055	CE1	PHE	263	53.539	29.584	97.182	1.00	20.00
ATOM	2056	CE2	PHE	263	52.427	28.148	98.713	1.00	20.00
ATOM	2057	CZ	PHE	263	53.333	28.327	97.695	1.00	20.00
ATOM	2058	C	PHE	263	49.066	30.674	98.520	1.00	20.00
ATOM	2059	O	PHE	263	48.600	30.378	99.618	1.00	20.00
ATOM	2060	N	GLY	264	48.807	29.940	97.425	1.00	20.00
ATOM	2061	CA	GLY	264	47.937	28.810	97.570	1.00	20.00
ATOM	2062	C	GLY	264	46.566	29.344	97.894	1.00	20.00
ATOM	2063	O	GLY	264	46.089	30.251	97.221	1.00	20.00
ATOM	2064	N	ALA	265	45.864	28.715	98.867	1.00	20.00
ATOM	2065	CA	ALA	265	44.568	29.095	99.377	1.00	20.00
ATOM	2066	CB	ALA	265	43.845	27.934	100.080	1.00	20.00
ATOM	2067	C	ALA	265	44.664	30.215	100.375	1.00	20.00
ATOM	2068	O	ALA	265	43.738	31.012	100.506	1.00	20.00
ATOM	2069	N	THR	266	45.779	30.280	101.130	1.00	20.00
ATOM	2070	CA	THR	266	45.922	31.197	102.231	1.00	20.00
ATOM	2071	CB	THR	266	46.519	30.528	103.439	1.00	20.00
ATOM	2072	OG1	THR	266	46.489	31.387	104.569	1.00	20.00
ATOM	2073	CG2	THR	266	47.970	30.135	103.111	1.00	20.00
ATOM	2074	C	THR	266	46.836	32.317	101.850	1.00	20.00
ATOM	2075	O	THR	266	47.360	32.360	100.738	1.00	20.00
ATOM	2076	N	CYS	267	47.017	33.281	102.777	1.00	20.00
ATOM	2077	CA	CYS	267	47.856	34.409	102.505	1.00	20.00
ATOM	2078	CB	CYS	267	47.107	35.736	102.555	1.00	20.00
ATOM	2079	SG	CYS	267	46.042	35.896	101.105	1.00	20.00

Figure 6 (continued)

ATOM	2080	C	CYS	267	48.973	34.484	103.496	1.00	20.00
ATOM	2081	O	CYS	267	48.868	33.985	104.616	1.00	20.00
ATOM	2082	N	VAL	268	50.090	35.112	103.072	1.00	20.00
ATOM	2083	CA	VAL	268	51.246	36.256	103.914	1.00	20.00
ATOM	2084	CB	VAL	268	52.450	34.530	103.389	1.00	20.00
ATOM	2085	CG1	VAL	268	53.613	34.767	104.364	1.00	20.00
ATOM	2086	CG2	VAL	268	52.092	33.068	103.198	1.00	20.00
ATOM	2087	C	VAL	268	51.585	36.715	103.960	1.00	20.00
ATOM	2088	O	VAL	268	51.367	37.444	102.991	1.00	20.00
ATOM	2089	N	LYS	269	52.113	37.182	105.112	1.00	20.00
ATOM	2090	CA	LYS	269	52.451	38.568	105.266	1.00	20.00
ATOM	2091	CB	LYS	269	52.897	38.932	106.691	1.00	20.00
ATOM	2092	CG	LYS	269	53.252	40.415	106.830	1.00	20.00
ATOM	2093	CD	LYS	269	52.054	41.348	106.639	1.00	20.00
ATOM	2094	CE	LYS	269	52.436	42.829	106.565	1.00	20.00
ATOM	2095	NZ	LYS	269	52.973	43.147	105.223	1.00	20.00
ATOM	2096	C	LYS	269	53.570	38.918	104.343	1.00	20.00
ATOM	2097	O	LYS	269	53.514	39.939	103.656	1.00	20.00
ATOM	2098	N	LYS	270	54.617	38.072	104.293	1.00	20.00
ATOM	2099	CA	LYS	270	55.742	38.377	103.458	1.00	20.00
ATOM	2100	CB	LYS	270	57.039	38.620	104.246	1.00	20.00
ATOM	2101	CG	LYS	270	56.941	39.777	105.244	1.00	20.00
ATOM	2102	CD	LYS	270	56.596	41.126	104.611	1.00	20.00
ATOM	2103	CE	LYS	270	56.481	42.265	105.627	1.00	20.00
ATOM	2104	NZ	LYS	270	56.117	43.527	104.941	1.00	20.00
ATOM	2105	C	LYS	270	55.960	37.190	102.584	1.00	20.00
ATOM	2106	O	LYS	270	55.479	36.096	102.855	1.00	20.00
ATOM	2107	N	CYS	271	56.716	37.390	101.486	1.00	20.00
ATOM	2108	CA	CYS	271	56.954	36.331	100.554	1.00	20.00
ATOM	2109	CB	CYS	271	57.366	36.914	99.198	1.00	20.00
ATOM	2110	SG	CYS	271	57.362	35.766	97.784	1.00	20.00
ATOM	2111	C	CYS	271	58.038	35.470	101.128	1.00	20.00
ATOM	2112	O	CYS	271	59.021	35.984	101.679	1.00	20.00
ATOM	2113	N	PRO	272	57.859	34.179	101.025	1.00	20.00
ATOM	2114	CA	PRO	272	58.826	33.259	101.566	1.00	20.00
ATOM	2115	CB	PRO	272	56.523	33.611	101.055	1.00	20.00
ATOM	2116	CB	PRO	272	58.117	31.907	101.681	1.00	20.00
ATOM	2117	CG	PRO	272	56.772	32.101	100.956	1.00	20.00
ATOM	2118	C	PRO	272	60.056	33.247	100.722	1.00	20.00
ATOM	2119	O	PRO	272	60.007	33.707	99.583	1.00	20.00
ATOM	2120	N	ARG	273	61.171	32.732	101.270	1.00	20.00
ATOM	2121	CA	ARG	273	62.413	32.734	100.559	1.00	20.00
ATOM	2122	CB	ARG	273	63.550	32.037	101.326	1.00	20.00
ATOM	2123	CG	ARG	273	64.913	32.136	100.638	1.00	20.00
ATOM	2124	CD	ARG	273	66.068	31.639	101.511	1.00	20.00
ATOM	2125	NE	ARG	273	65.997	30.152	101.561	1.00	20.00
ATOM	2126	CZ	ARG	273	66.655	29.407	100.625	1.00	20.00
ATOM	2127	NH1	ARG	273	67.376	30.026	99.645	1.00	20.00
ATOM	2128	NH2	ARG	273	66.595	28.084	100.672	1.00	20.00
ATOM	2129	C	ARG	273	62.202	32.027	99.262	1.00	20.00
ATOM	2130	O	ARG	273	61.289	31.216	99.133	1.00	20.00
ATOM	2131	N	ASN	274	63.045	32.370	98.265	1.00	20.00
ATOM	2132	CA	ASN	274	63.051	31.844	96.926	1.00	20.00
ATOM	2133	CB	ASN	274	63.505	30.369	96.793	1.00	20.00
ATOM	2134	CG	ASN	274	62.563	29.415	97.519	1.00	20.00
ATOM	2135	OD1	ASN	274	62.809	29.031	98.661	1.00	20.00
ATOM	2136	ND2	ASN	274	61.448	29.024	96.845	1.00	20.00
ATOM	2137	C	ASN	274	61.712	32.030	96.278	1.00	20.00
ATOM	2138	O	ASN	274	61.392	31.258	95.402	1.00	20.00
ATOM	2139	N	TYR	275	60.979	33.086	96.585	1.00	20.00
ATOM	2140	CA	TYR	275	59.712	33.421	96.095	1.00	20.00
ATOM	2141	CB	TYR	275	58.493	33.076	96.975	1.00	20.00
ATOM	2142	CG	TYR	275	58.268	31.602	96.996	1.00	20.00
ATOM	2143	CD1	TYR	275	57.473	31.010	96.042	1.00	20.00
ATOM	2144	CD2	TYR	275	58.838	30.812	97.965	1.00	20.00
ATOM	2145	CE1	TYR	275	57.252	29.653	96.049	1.00	20.00
ATOM	2146	CE2	TYR	275	58.623	29.454	97.980	1.00	20.00
ATOM	2147	CZ	TYR	275	57.830	28.872	97.020	1.00	20.00
ATOM	2148	OH	TYR	275	57.608	27.477	97.034	1.00	20.00
ATOM	2149	C	TYR	275	59.716	34.909	95.932	1.00	20.00
ATOM	2150	O	TYR	275	60.361	35.621	96.698	1.00	20.00
ATOM	2151	N	VAL	276	58.988	35.421	94.920	1.00	20.00
ATOM	2152	CA	VAL	276	58.972	36.835	94.683	1.00	20.00
ATOM	2153	CB	VAL	276	59.460	37.200	93.315	1.00	20.00
ATOM	2154	CG1	VAL	276	60.930	36.768	93.186	1.00	20.00
ATOM	2155	CG2	VAL	276	58.525	36.544	92.285	1.00	20.00
ATOM	2156	C	VAL	276	57.553	37.302	94.770	1.00	20.00

Figure 6 (continued)

ATOM	2157	C	VAL	276	56.618	36.514	94.641	1.00 20.00
ATOM	2158	N	VAL	277	57.362	38.614	95.011	1.00 20.00
ATOM	2159	CA	VAL	277	56.037	39.162	95.109	1.00 20.00
ATOM	2160	CB	VAL	277	55.890	40.173	96.197	1.00 20.00
ATOM	2161	CG1	VAL	277	54.450	40.714	96.171	1.00 20.00
ATOM	2162	CG2	VAL	277	56.288	39.520	97.534	1.00 20.00
ATOM	2163	C	VAL	277	55.745	39.832	93.818	1.00 20.00
ATOM	2164	O	VAL	277	56.453	40.754	93.420	1.00 20.00
ATOM	2165	N	THR	278	54.679	39.389	93.154	1.00 20.00
ATOM	2166	CA	THR	278	54.407	39.977	91.852	1.00 20.00
ATOM	2167	CB	THR	278	54.585	39.022	90.709	1.00 20.00
ATOM	2168	OG1	THR	278	55.915	38.522	90.691	1.00 20.00
ATOM	2169	CG2	THR	278	54.287	39.766	89.396	1.00 20.00
ATOM	2170	C	THR	278	52.998	40.458	91.817	1.00 20.00
ATOM	2171	O	THR	278	52.111	39.887	92.450	1.00 20.00
ATOM	2172	N	ASP	279	52.777	41.551	91.063	1.00 20.00
ATOM	2173	CA	ASP	279	51.474	42.111	90.851	1.00 20.00
ATOM	2174	CB	ASP	279	50.531	41.179	90.103	1.00 20.00
ATOM	2175	CG	ASP	279	51.055	41.088	88.679	1.00 20.00
ATOM	2176	OD1	ASP	279	51.507	42.139	88.152	1.00 20.00
ATOM	2177	OD2	ASP	279	51.023	39.967	88.104	1.00 20.00
ATOM	2178	C	ASP	279	50.875	42.370	92.215	1.00 20.00
ATOM	2179	O	ASP	279	49.674	42.165	92.391	1.00 20.00
ATOM	2180	N	HIS	280	51.717	42.851	93.156	1.00 20.00
ATOM	2181	CA	HIS	280	51.368	43.212	94.502	1.00 20.00
ATOM	2182	ND1	HIS	280	52.070	46.097	92.921	1.00 20.00
ATOM	2183	NE2	HIS	280	53.524	47.211	94.187	1.00 20.00
ATOM	2184	CE1	HIS	280	53.071	47.013	92.959	1.00 20.00
ATOM	2185	CD2	HIS	280	52.764	46.369	94.976	1.00 20.00
ATOM	2186	CG	HIS	280	51.860	45.679	94.219	1.00 20.00
ATOM	2187	CB	HIS	280	50.849	44.657	94.624	1.00 20.00
ATOM	2188	C	HIS	280	50.317	42.294	95.034	1.00 20.00
ATOM	2189	O	HIS	280	49.125	42.521	94.835	1.00 20.00
ATOM	2190	N	GLY	281	50.720	41.240	95.766	1.00 20.00
ATOM	2191	CA	GLY	281	49.688	40.384	96.265	1.00 20.00
ATOM	2192	C	GLY	281	49.950	39.953	95.920	1.00 20.00
ATOM	2193	O	GLY	281	49.344	38.064	96.512	1.00 20.00
ATOM	2194	N	SER	282	50.823	38.648	94.949	1.00 20.00
ATOM	2195	CA	SER	282	51.016	37.241	94.763	1.00 20.00
ATOM	2196	CB	SER	282	50.689	36.754	93.340	1.00 20.00
ATOM	2197	OG	SER	282	50.912	35.356	93.242	1.00 20.00
ATOM	2198	C	SER	282	52.458	36.940	95.009	1.00 20.00
ATOM	2199	O	SER	282	53.346	37.526	94.393	1.00 20.00
ATOM	2200	N	CYS	283	52.727	36.015	95.947	1.00 20.00
ATOM	2201	CA	CYS	283	54.070	35.598	96.216	1.00 20.00
ATOM	2202	CB	CYS	283	54.318	35.411	97.723	1.00 20.00
ATOM	2203	SG	CYS	283	55.825	34.499	98.162	1.00 20.00
ATOM	2204	C	CYS	283	54.204	34.280	95.544	1.00 20.00
ATOM	2205	O	CYS	283	53.664	33.273	95.999	1.00 20.00
ATOM	2206	N	VAL	284	54.924	34.272	94.411	1.00 20.00
ATOM	2207	CA	VAL	284	55.105	33.072	93.660	1.00 20.00
ATOM	2208	CB	VAL	284	54.524	33.155	92.280	1.00 20.00
ATOM	2209	CG1	VAL	284	55.139	34.372	91.571	1.00 20.00
ATOM	2210	CG2	VAL	284	54.771	31.820	91.558	1.00 20.00
ATOM	2211	C	VAL	284	56.574	32.850	93.542	1.00 20.00
ATOM	2212	O	VAL	284	57.366	33.781	93.672	1.00 20.00
ATOM	2213	N	ARG	285	56.977	31.587	93.311	1.00 20.00
ATOM	2214	CA	ARG	285	58.372	31.270	93.249	1.00 20.00
ATOM	2215	CB	ARG	285	58.665	29.774	93.046	1.00 20.00
ATOM	2216	CG	ARG	285	60.167	29.484	92.987	1.00 20.00
ATOM	2217	CD	ARG	285	60.519	28.046	92.605	1.00 20.00
ATOM	2218	NE	ARG	285	60.007	27.152	93.680	1.00 20.00
ATOM	2219	CZ	ARG	285	60.487	25.879	93.789	1.00 20.00
ATOM	2220	NH1	ARG	285	61.467	25.446	92.942	1.00 20.00
ATOM	2221	NH2	ARG	285	59.989	25.040	94.743	1.00 20.00
ATOM	2222	C	ARG	285	58.996	31.986	92.101	1.00 20.00
ATOM	2223	O	ARG	285	60.115	32.481	92.219	1.00 20.00
ATOM	2224	N	ALA	286	58.299	32.062	90.951	1.00 20.00
ATOM	2225	CA	ALA	286	58.919	32.693	89.823	1.00 20.00
ATOM	2226	CB	ALA	286	59.147	31.737	88.641	1.00 20.00
ATOM	2227	C	ALA	286	58.041	33.793	89.334	1.00 20.00
ATOM	2228	O	ALA	286	56.823	33.767	89.497	1.00 20.00
ATOM	2229	N	CYS	287	58.663	34.801	88.698	1.00 20.00
ATOM	2230	CA	CYS	287	57.932	35.932	88.223	1.00 20.00
ATOM	2231	CB	CYS	287	58.821	37.146	88.001	1.00 20.00
ATOM	2232	SG	CYS	287	59.371	37.729	89.624	1.00 20.00
ATOM	2233	C	CYS	287	57.220	35.562	86.973	1.00 20.00

Figure 6 (continued)

ATOM	2234	O	CYS	287	57.434	34.486	86.416	1.00	20.00
ATOM	2235	N	GLY	288	56.313	36.450	86.526	1.00	20.00
ATOM	2236	CA	GLY	288	55.567	36.180	85.339	1.00	20.00
ATOM	2237	C	GLY	288	56.571	36.093	84.235	1.00	20.00
ATOM	2238	O	GLY	288	57.707	36.543	84.371	1.00	20.00
ATOM	2239	N	ALA	289	56.147	35.526	83.091	1.00	20.00
ATOM	2240	CA	ALA	289	57.019	35.255	81.986	1.00	20.00
ATOM	2241	CB	ALA	289	56.254	34.835	80.719	1.00	20.00
ATOM	2242	C	ALA	289	57.856	36.445	81.630	1.00	20.00
ATOM	2243	O	ALA	289	59.054	36.465	81.896	1.00	20.00
ATOM	2244	N	ASP	290	57.232	37.480	81.038	1.00	20.00
ATOM	2245	CA	ASP	290	57.915	38.634	80.522	1.00	20.00
ATOM	2246	CB	ASP	290	56.966	39.629	79.835	1.00	20.00
ATOM	2247	CG	ASP	290	56.517	39.010	78.519	1.00	20.00
ATOM	2248	OD1	ASP	290	57.304	38.210	77.945	1.00	20.00
ATOM	2249	OD2	ASP	290	55.383	39.326	78.071	1.00	20.00
ATOM	2250	C	ASP	290	58.629	39.366	81.613	1.00	20.00
ATOM	2251	O	ASP	290	59.445	40.242	81.327	1.00	20.00
ATOM	2252	N	SER	291	58.343	39.063	82.892	1.00	20.00
ATOM	2253	CA	SER	291	58.974	39.873	83.937	1.00	20.00
ATOM	2254	CB	SER	291	58.083	39.996	85.177	1.00	20.00
ATOM	2255	OG	SER	291	57.857	38.735	85.790	1.00	20.00
ATOM	2256	C	SER	291	60.230	39.147	84.393	1.00	20.00
ATOM	2257	O	SER	291	60.313	37.920	84.434	1.00	20.00
ATOM	2258	N	TYR	292	61.260	39.953	84.740	1.00	20.00
ATOM	2259	CA	TYR	292	62.483	39.388	85.236	1.00	20.00
ATOM	2260	CB	TYR	292	63.702	39.590	84.319	1.00	20.00
ATOM	2261	CG	TYR	292	64.847	38.888	84.968	1.00	20.00
ATOM	2262	CD1	TYR	292	64.939	37.514	84.919	1.00	20.00
ATOM	2263	CD2	TYR	292	65.832	39.596	85.616	1.00	20.00
ATOM	2264	CE1	TYR	292	65.991	36.857	85.512	1.00	20.00
ATOM	2265	CE2	TYR	292	66.887	38.945	86.210	1.00	20.00
ATOM	2266	CZ	TYR	292	66.966	37.574	86.160	1.00	20.00
ATOM	2267	OH	TYR	292	68.047	36.903	86.772	1.00	20.00
ATOM	2268	C	TYR	292	62.771	40.031	86.558	1.00	20.00
ATOM	2269	O	TYR	292	62.343	41.153	86.827	1.00	20.00
ATOM	2270	N	GLU	293	63.506	39.310	87.424	1.00	20.00
ATOM	2271	CA	GLU	293	63.817	39.765	88.747	1.00	20.00
ATOM	2272	CB	GLU	293	64.760	38.802	89.492	1.00	20.00
ATOM	2273	CG	GLU	293	64.180	37.407	89.727	1.00	20.00
ATOM	2274	CD	GLU	293	65.318	36.507	90.193	1.00	20.00
ATOM	2275	OE1	GLU	293	66.481	36.755	89.775	1.00	20.00
ATOM	2276	OE2	GLU	293	65.040	35.559	90.975	1.00	20.00
ATOM	2277	C	GLU	293	64.542	41.062	88.625	1.00	20.00
ATOM	2278	O	GLU	293	65.427	41.219	87.788	1.00	20.00
ATOM	2279	N	MET	294	64.173	42.042	89.468	1.00	20.00
ATOM	2280	CA	MET	294	64.826	43.315	89.429	1.00	20.00
ATOM	2281	CB	MET	294	64.217	44.319	90.420	1.00	20.00
ATOM	2282	CG	MET	294	64.869	45.702	90.379	1.00	20.00
ATOM	2283	SD	MET	294	64.156	46.897	91.550	1.00	20.00
ATOM	2284	CE	MET	294	65.245	48.265	91.060	1.00	20.00
ATOM	2285	C	MET	294	66.261	43.095	89.822	1.00	20.00
ATOM	2286	O	MET	294	67.168	43.650	89.218	1.00	20.00
ATOM	2287	N	GLU	295	66.474	42.249	90.844	1.00	40.00
ATOM	2288	CA	GLU	295	67.805	42.008	91.314	1.00	40.00
ATOM	2289	CB	GLU	295	68.039	42.506	92.750	1.00	40.00
ATOM	2290	CG	GLU	295	67.891	44.022	92.895	1.00	40.00
ATOM	2291	CD	GLU	295	69.035	44.691	92.148	1.00	40.00
ATOM	2292	OE1	GLU	295	70.192	44.615	92.642	1.00	40.00
ATOM	2293	OE2	GLU	295	68.767	45.289	91.072	1.00	40.00
ATOM	2294	C	GLU	295	67.994	40.529	91.327	1.00	40.00
ATOM	2295	O	GLU	295	67.235	39.788	90.707	1.00	40.00
ATOM	2296	N	GLU	296	69.037	40.054	92.037	1.00	40.00
ATOM	2297	CA	GLU	296	69.282	38.644	92.111	1.00	40.00
ATOM	2298	CB	GLU	296	70.540	38.261	92.910	1.00	40.00
ATOM	2299	CG	GLU	296	71.859	38.629	92.226	1.00	40.00
ATOM	2300	CD	GLU	296	72.137	40.107	92.460	1.00	40.00
ATOM	2301	OE1	GLU	296	71.486	40.950	91.786	1.00	40.00
ATOM	2302	OE2	GLU	296	73.008	40.413	93.317	1.00	40.00
ATOM	2303	C	GLU	296	68.118	38.016	92.802	1.00	40.00
ATOM	2304	O	GLU	296	67.159	38.693	93.168	1.00	40.00
ATOM	2305	N	ASP	297	68.183	36.684	92.990	1.00	40.00
ATOM	2306	CA	ASP	297	67.104	35.969	93.604	1.00	40.00
ATOM	2307	CB	ASP	297	67.407	34.485	93.883	1.00	40.00
ATOM	2308	CG	ASP	297	66.533	34.410	94.905	1.00	40.00
ATOM	2309	OD1	ASP	297	69.311	35.396	95.007	1.00	40.00
ATOM	2310	OD2	ASP	297	68.625	33.365	95.604	1.00	40.00

Figure 6 (continued)

ATOM	2311	C	ASP	297	66.807	36.618	94.909	1.00	40.00
ATOM	2312	O	ASP	297	67.661	37.271	95.505	1.00	40.00
ATOM	2313	N	GLY	298	65.555	36.477	95.372	1.00	40.00
ATOM	2314	CA	GLY	298	65.194	37.090	96.609	1.00	40.00
ATOM	2315	C	GLY	298	64.645	38.494	96.276	1.00	40.00
ATOM	2316	O	GLY	298	63.967	39.056	97.091	1.00	40.00
ATOM	2317	N	VAL	299	64.926	38.924	95.052	1.00	40.00
ATOM	2318	CA	VAL	299	64.378	40.198	94.705	1.00	40.00
ATOM	2319	CB	VAL	299	64.782	40.690	93.341	1.00	40.00
ATOM	2320	CG1	VAL	299	64.331	39.674	92.277	1.00	40.00
ATOM	2321	CG2	VAL	299	64.195	42.098	93.142	1.00	40.00
ATOM	2322	C	VAL	299	62.898	40.020	94.753	1.00	40.00
ATOM	2323	O	VAL	299	62.330	39.173	94.078	1.00	40.00
ATOM	2324	N	ARG	300	62.237	40.824	95.600	1.00	40.00
ATOM	2325	CA	ARG	300	60.821	40.703	95.771	1.00	40.00
ATOM	2326	CB	ARG	300	60.278	41.579	96.912	1.00	40.00
ATOM	2327	CG	ARG	300	60.740	41.130	98.298	1.00	40.00
ATOM	2328	CD	ARG	300	60.201	41.999	99.436	1.00	40.00
ATOM	2329	NE	ARG	300	60.665	41.392	100.714	1.00	40.00
ATOM	2330	CZ	ARG	300	59.910	40.425	101.313	1.00	40.00
ATOM	2331	NH1	ARG	300	58.740	40.020	100.739	1.00	40.00
ATOM	2332	NH2	ARG	300	60.323	39.863	102.486	1.00	40.00
ATOM	2333	C	ARG	300	60.124	41.135	94.527	1.00	40.00
ATOM	2334	O	ARG	300	59.193	40.474	94.069	1.00	40.00
ATOM	2335	N	LYS	301	60.575	42.252	93.927	1.00	20.00
ATOM	2336	CA	LYS	301	59.934	42.778	92.822	1.00	20.00
ATOM	2337	CB	LYS	301	59.763	44.316	92.798	1.00	20.00
ATOM	2338	CG	LYS	301	58.943	44.919	93.961	1.00	20.00
ATOM	2339	CD	LYS	301	59.127	46.431	94.097	1.00	20.00
ATOM	2340	CE	LYS	301	58.320	47.032	95.251	1.00	20.00
ATOM	2341	NZ	LYS	301	58.597	48.482	95.362	1.00	20.00
ATOM	2342	C	LYS	301	60.485	42.360	91.538	1.00	20.00
ATOM	2343	O	LYS	301	61.671	42.221	91.417	1.00	20.00
ATOM	2344	N	CYS	302	59.590	42.113	90.540	1.00	20.00
ATOM	2345	CA	CYS	302	60.075	41.810	89.236	1.00	20.00
ATOM	2346	CB	CYS	302	59.698	40.492	88.646	1.00	20.00
ATOM	2347	SG	CYS	302	60.700	39.150	89.141	1.00	20.00
ATOM	2348	C	CYS	302	59.652	42.918	88.338	1.00	20.00
ATOM	2349	O	CYS	302	58.613	43.540	88.645	1.00	20.00
ATOM	2350	N	LYS	303	60.484	43.194	87.320	1.00	20.00
ATOM	2351	CA	LYS	303	60.197	44.260	86.423	1.00	20.00
ATOM	2352	CB	LYS	303	61.373	45.234	86.238	1.00	20.00
ATOM	2353	CG	LYS	303	62.526	44.582	85.452	1.00	20.00
ATOM	2354	CD	LYS	303	63.533	45.572	84.864	1.00	20.00
ATOM	2355	CE	LYS	303	64.622	44.898	84.026	1.00	20.00
ATOM	2356	NZ	LYS	303	65.408	45.921	83.300	1.00	20.00
ATOM	2357	C	LYS	303	59.942	43.671	85.081	1.00	20.00
ATOM	2358	O	LYS	303	60.253	42.506	84.837	1.00	20.00
ATOM	2359	N	LYS	304	59.351	44.469	84.170	1.00	20.00
ATOM	2360	CA	LYS	304	59.076	43.986	82.860	1.00	20.00
ATOM	2361	CB	LYS	304	57.951	44.714	82.194	1.00	20.00
ATOM	2362	CG	LYS	304	57.601	44.010	80.842	1.00	20.00
ATOM	2363	CD	LYS	304	56.098	44.414	80.381	1.00	20.00
ATOM	2364	CE	LYS	304	55.807	45.906	80.526	1.00	20.00
ATOM	2365	NZ	LYS	304	56.339	46.645	79.364	1.00	20.00
ATOM	2366	C	LYS	304	60.333	44.013	82.062	1.00	20.00
ATOM	2367	O	LYS	304	61.229	44.813	82.327	1.00	20.00
ATOM	2368	N	CYS	305	60.426	43.120	81.060	1.00	20.00
ATOM	2369	CA	CYS	305	61.605	43.022	80.255	1.00	20.00
ATOM	2370	CB	CYS	305	61.923	41.576	79.836	1.00	20.00
ATOM	2371	SG	CYS	305	62.261	40.466	81.234	1.00	20.00
ATOM	2372	C	CYS	305	61.348	43.763	78.990	1.00	20.00
ATOM	2373	O	CYS	305	60.357	43.515	78.304	1.00	20.00
ATOM	2374	N	GLU	306	62.237	44.713	78.647	1.00	20.00
ATOM	2375	CA	GLU	306	62.038	45.388	77.405	1.00	20.00
ATOM	2376	CB	GLU	306	63.069	46.499	77.143	1.00	20.00
ATOM	2377	CG	GLU	306	62.966	47.682	78.108	1.00	20.00
ATOM	2378	CD	GLU	306	64.070	48.668	77.755	1.00	20.00
ATOM	2379	OE1	GLU	306	65.025	48.253	77.046	1.00	20.00
ATOM	2380	OE2	GLU	306	63.975	49.847	78.191	1.00	20.00
ATOM	2381	C	GLU	306	62.236	44.363	76.362	1.00	20.00
ATOM	2382	O	GLU	306	63.354	43.882	76.138	1.00	20.00
ATOM	2383	N	GLY	307	61.141	43.941	75.690	1.00	20.00
ATOM	2384	CA	GLY	307	61.249	42.931	74.680	1.00	20.00
ATOM	2385	C	GLY	307	61.336	41.605	75.359	1.00	20.00
ATOM	2386	O	GLY	307	60.880	41.425	76.487	1.00	20.00
ATOM	2387	N	PRO	308	61.915	40.663	74.674	1.00	20.00

Figure 6 (continued)

ATOM	2388	CA	PRO	308	62.045	39.363	75.260	1.00	20.00
ATOM	2389	CD	PRO	308	61.778	40.595	73.229	1.00	20.00
ATOM	2390	CB	PRO	308	62.453	38.433	74.123	1.00	20.00
ATOM	2391	CG	PRO	308	61.825	39.057	72.882	1.00	20.00
ATOM	2392	C	PRO	308	63.008	39.464	76.395	1.00	20.00
ATOM	2393	O	PRO	308	63.960	40.219	76.315	1.00	20.00
ATOM	2394	N	CYS	309	62.782	38.656	77.461	1.00	20.00
ATOM	2395	CA	CYS	309	63.646	38.731	78.600	1.00	20.00
ATOM	2396	CB	CYS	309	63.155	37.947	79.827	1.00	20.00
ATOM	2397	SG	CYS	309	61.647	38.660	80.535	1.00	20.00
ATOM	2398	C	CYS	309	64.968	38.170	78.213	1.00	20.00
ATOM	2399	O	CYS	309	65.075	37.383	77.274	1.00	20.00
ATOM	2400	N	ARG	310	66.001	38.587	78.939	1.00	20.00
ATOM	2401	CA	ARG	310	67.329	38.103	78.638	1.00	20.00
ATOM	2402	CB	ARG	310	68.455	38.788	79.429	1.00	20.00
ATOM	2403	CG	ARG	310	68.714	40.248	79.060	1.00	20.00
ATOM	2404	CD	ARG	310	69.852	40.857	79.880	1.00	20.00
ATOM	2405	NE	ARG	310	70.033	42.269	79.445	1.00	20.00
ATOM	2406	CZ	ARG	310	70.714	43.137	80.248	1.00	20.00
ATOM	2407	NH1	ARG	310	71.198	42.711	81.451	1.00	20.00
ATOM	2408	NH2	ARG	310	70.907	44.428	79.051	1.00	20.00
ATOM	2409	C	ARG	310	67.381	36.665	79.018	1.00	20.00
ATOM	2410	O	ARG	310	66.769	36.240	79.998	1.00	20.00
ATOM	2411	N	LYS	311	68.135	35.874	78.210	1.00	20.00
ATOM	2412	CA	LYS	311	68.309	34.493	78.507	1.00	20.00
ATOM	2413	CB	LYS	311	67.442	33.646	77.659	1.00	20.00
ATOM	2414	CG	LYS	311	67.695	33.660	76.155	1.00	20.00
ATOM	2415	CD	LYS	311	67.052	32.535	75.341	1.00	20.00
ATOM	2416	CE	LYS	311	65.524	32.595	75.322	1.00	20.00
ATOM	2417	NZ	LYS	311	64.982	31.475	74.516	1.00	20.00
ATOM	2418	C	LYS	311	69.739	34.229	78.170	1.00	20.00
ATOM	2419	O	LYS	311	70.274	34.799	77.221	1.00	20.00
ATOM	2420	N	VAL	312	70.408	33.369	78.957	1.00	20.00
ATOM	2421	CA	VAL	312	71.785	33.090	78.680	1.00	20.00
ATOM	2422	CB	VAL	312	72.524	32.834	79.860	1.00	20.00
ATOM	2423	CG1	VAL	312	72.548	33.595	80.972	1.00	20.00
ATOM	2424	CG2	VAL	312	71.850	31.214	80.272	1.00	20.00
ATOM	2425	C	VAL	312	71.810	32.027	77.590	1.00	20.00
ATOM	2426	O	VAL	312	70.709	31.582	77.169	1.00	20.00
ATOM	2427	OXT	VAL	312	72.933	31.643	77.168	1.00	20.00
TER									
ATOM	1	N	CYS	313	73.141	29.695	76.381	1.00	40.00
ATOM	2	CA	CYS	313	73.419	28.319	76.901	1.00	40.00
ATOM	3	C	CYS	313	74.891	28.025	76.031	1.00	40.00
ATOM	4	O	CYS	313	75.701	28.940	75.935	1.00	40.00
ATOM	5	CB	CYS	313	72.951	28.209	74.438	1.00	40.00
ATOM	6	SG	CYS	313	71.140	28.384	74.330	1.00	40.00
ATOM	7	N	ASN	314	75.288	26.752	76.281	1.00	40.00
ATOM	8	CA	ASN	314	76.686	26.424	76.461	1.00	40.00
ATOM	9	C	ASN	314	77.304	26.180	75.118	1.00	40.00
ATOM	10	O	ASN	314	76.621	26.277	74.100	1.00	40.00
ATOM	11	CB	ASN	314	76.926	25.170	77.321	1.00	40.00
ATOM	12	CG	ASN	314	76.570	25.510	78.763	1.00	40.00
ATOM	13	OD1	ASN	314	76.310	26.665	79.098	1.00	40.00
ATOM	14	ND2	ASN	314	76.566	24.476	79.646	1.00	40.00
ATOM	15	N	GLY	315	78.627	25.876	75.097	1.00	40.00
ATOM	16	CA	GLY	315	79.353	25.621	73.879	1.00	40.00
ATOM	17	C	GLY	315	78.558	24.619	73.123	1.00	40.00
ATOM	18	O	GLY	315	78.278	23.531	73.622	1.00	40.00
ATOM	19	N	ILE	316	78.173	24.968	71.884	1.00	40.00
ATOM	20	CA	ILE	316	77.311	24.088	71.163	1.00	40.00
ATOM	21	C	ILE	316	78.041	23.538	69.985	1.00	40.00
ATOM	22	O	ILE	316	78.765	24.250	69.291	1.00	40.00
ATOM	23	CB	ILE	316	76.080	24.780	70.659	1.00	40.00
ATOM	24	CG1	ILE	316	75.286	25.360	71.842	1.00	40.00
ATOM	25	CG2	ILE	316	75.280	23.781	69.805	1.00	40.00
ATOM	26	CD1	ILE	316	74.190	26.340	71.429	1.00	40.00
ATOM	27	N	GLY	317	77.876	22.223	69.747	1.00	40.00
ATOM	28	CA	GLY	317	78.486	21.627	68.598	1.00	40.00
ATOM	29	C	GLY	317	77.374	21.042	67.793	1.00	40.00
ATOM	30	O	GLY	317	76.969	19.900	68.006	1.00	40.00
ATOM	31	N	ILE	318	76.870	21.823	66.820	1.00	40.00
ATOM	32	CA	ILE	318	75.788	21.390	65.989	1.00	40.00
ATOM	33	C	ILE	318	76.396	20.564	64.903	1.00	40.00
ATOM	34	O	ILE	318	77.604	20.613	64.678	1.00	40.00
ATOM	35	CB	ILE	318	75.047	22.550	65.370	1.00	40.00
ATOM	36	CG1	ILE	318	74.531	23.485	66.475	1.00	40.00

Figure 6 (continued)

ATOM	37	CG2	ILE	318	73.908	22.013	64.486	1.00 40.00
ATOM	38	CD1	ILE	318	73.552	22.811	67.434	1.00 40.00
ATOM	39	N	GLY	319	75.571	19.755	64.212	1.00 40.00
ATOM	40	CA	GLY	319	76.088	18.939	63.155	1.00 40.00
ATOM	41	C	GLY	319	76.427	17.606	63.734	1.00 40.00
ATOM	42	O	GLY	319	76.272	17.374	64.932	1.00 40.00
ATOM	43	N	GLU	320	76.901	16.690	62.869	1.00 40.00
ATOM	44	CA	GLU	320	77.247	15.367	63.294	1.00 40.00
ATOM	45	C	GLU	320	76.718	15.216	63.107	1.00 40.00
ATOM	46	O	GLU	320	79.383	16.103	62.573	1.00 40.00
ATOM	47	CB	GLU	320	76.570	14.257	62.473	1.00 40.00
ATOM	48	CG	GLU	320	76.058	14.197	62.694	1.00 40.00
ATOM	49	CD	GLU	320	74.817	13.615	64.083	1.00 40.00
ATOM	50	OE1	GLU	320	75.209	12.439	64.312	1.00 40.00
ATOM	51	OE2	GLU	320	74.242	14.343	64.934	1.00 40.00
ATOM	52	N	PHE	321	79.270	14.681	63.574	1.00 60.00
ATOM	53	CA	PHE	321	80.678	13.870	63.447	1.00 60.00
ATOM	54	C	PHE	321	81.006	13.918	61.993	1.00 60.00
ATOM	55	O	PHE	321	80.186	13.574	61.144	1.00 60.00
ATOM	56	CB	PHE	321	81.158	12.514	63.994	1.00 60.00
ATOM	57	CG	PHE	321	80.977	12.521	65.474	1.00 60.00
ATOM	58	CD1	PHE	321	79.764	12.188	66.031	1.00 60.00
ATOM	59	CD2	PHE	321	82.020	12.858	66.305	1.00 60.00
ATOM	60	CE1	PHE	321	79.595	12.192	67.397	1.00 60.00
ATOM	61	CE2	PHE	321	81.858	12.864	67.670	1.00 60.00
ATOM	62	CZ	PHE	321	80.642	12.531	68.219	1.00 60.00
ATOM	63	N	LYS	322	82.230	14.378	61.679	1.00 60.00
ATOM	64	CA	LYS	322	82.658	14.500	60.319	1.00 60.00
ATOM	65	C	LYS	322	87.709	13.137	59.717	1.00 60.00
ATOM	66	O	LYS	322	87.299	12.937	58.575	1.00 60.00
ATOM	67	CB	LYS	322	84.067	15.103	60.187	1.00 60.00
ATOM	68	CG	LYS	322	85.161	14.293	60.795	1.00 60.00
ATOM	69	CD	LYS	322	86.576	14.625	60.377	1.00 60.00
ATOM	70	CE	LYS	322	87.666	13.743	60.989	1.00 60.00
ATOM	71	NZ	LYS	322	89.000	14.195	60.533	1.00 60.00
ATOM	72	N	ASP	323	83.210	12.152	60.484	1.00 60.00
ATOM	73	CA	ASP	323	83.348	10.833	59.946	1.00 60.00
ATOM	74	C	ASP	323	81.994	10.353	59.549	1.00 60.00
ATOM	75	O	ASP	323	81.817	9.818	58.455	1.00 60.00
ATOM	76	CB	ASP	323	83.924	9.827	60.961	1.00 60.00
ATOM	77	CG	ASP	323	84.217	8.514	60.245	1.00 60.00
ATOM	78	OD1	ASP	323	84.830	8.377	59.054	1.00 60.00
ATOM	79	OD2	ASP	323	84.835	7.624	60.888	1.00 60.00
ATOM	80	N	SER	324	80.988	10.546	60.419	1.00 60.00
ATOM	81	CA	SER	324	79.691	10.070	60.094	1.00 60.00
ATOM	82	C	SER	324	79.241	10.862	58.874	1.00 60.00
ATOM	83	O	SER	324	79.250	12.091	58.894	1.00 60.00
ATOM	84	CB	SER	324	78.635	10.219	61.183	1.00 60.00
ATOM	85	OG	SER	324	78.416	11.592	61.453	1.00 60.00
ATOM	86	N	LEU	325	78.851	10.156	57.796	1.00 60.00
ATOM	87	CA	LEU	325	78.392	10.817	56.614	1.00 60.00
ATOM	88	C	LEU	325	77.121	11.514	56.961	1.00 60.00
ATOM	89	O	LEU	325	76.893	12.652	56.555	1.00 60.00
ATOM	90	CB	LEU	325	78.086	9.846	55.458	1.00 60.00
ATOM	91	CG	LEU	325	79.330	9.127	54.907	1.00 60.00
ATOM	92	CD1	LEU	325	80.303	10.118	54.249	1.00 60.00
ATOM	93	CD2	LEU	325	79.998	8.257	55.903	1.00 60.00
ATOM	94	N	SER	326	76.262	10.841	57.746	1.00 60.00
ATOM	95	CA	SER	326	75.004	11.425	58.094	1.00 60.00
ATOM	96	C	SER	326	75.270	12.652	58.895	1.00 60.00
ATOM	97	O	SER	326	76.143	12.672	59.762	1.00 60.00
ATOM	98	CB	SER	326	74.111	10.504	58.942	1.00 60.00
ATOM	99	OG	SER	326	74.705	10.289	60.215	1.00 60.00
ATOM	100	N	ILE	327	74.516	13.727	58.600	1.00 60.00
ATOM	101	CA	ILE	327	74.664	14.952	59.323	1.00 60.00
ATOM	102	C	ILE	327	73.323	15.261	59.890	1.00 60.00
ATOM	103	O	ILE	327	72.301	14.971	59.270	1.00 60.00
ATOM	104	CB	ILE	327	75.059	16.121	58.465	1.00 60.00
ATOM	105	CG1	ILE	327	73.974	16.438	57.418	1.00 60.00
ATOM	106	CG2	ILE	327	76.433	15.806	57.851	1.00 60.00
ATOM	107	CD1	ILE	327	73.735	15.320	56.404	1.00 60.00
ATOM	108	N	ASN	328	73.283	15.840	61.105	1.00 40.00
ATOM	109	CA	ASN	328	72.004	16.147	61.667	1.00 40.00
ATOM	110	C	ASN	328	71.761	17.606	61.479	1.00 40.00
ATOM	111	O	ASN	328	72.239	18.439	62.248	1.00 40.00
ATOM	112	CB	ASN	328	71.899	15.849	63.172	1.00 40.00
ATOM	113	CG	ASN	328	71.874	14.337	63.352	1.00 40.00

Figure 6 (continued)

ATOM	114	OD1	ASN	328	71.796	13.832	64.471	1.00	40.00
ATOM	115	ND2	ASN	328	71.943	13.591	62.217	1.00	40.00
ATOM	116	N	ALA	329	71.003	17.944	60.421	1.00	40.00
ATOM	117	CA	ALA	329	70.649	19.301	60.133	1.00	40.00
ATOM	118	C	ALA	329	69.694	19.720	61.196	1.00	40.00
ATOM	119	O	ALA	329	69.693	20.870	61.633	1.00	40.00
ATOM	120	CB	ALA	329	69.934	19.457	58.780	1.00	40.00
ATOM	121	N	THR	330	68.893	18.753	61.672	1.00	40.00
ATOM	122	CA	THR	330	67.833	18.948	62.619	1.00	40.00
ATOM	123	C	THR	330	68.393	19.563	63.859	1.00	40.00
ATOM	124	O	THR	330	67.671	20.212	64.612	1.00	40.00
ATOM	125	CB	THR	330	67.171	17.662	63.016	1.00	40.00
ATOM	126	OG1	THR	330	66.028	17.923	63.816	1.00	40.00
ATOM	127	CG2	THR	330	68.183	16.804	63.794	1.00	40.00
ATOM	128	N	ASN	331	69.699	19.365	64.098	1.00	40.00
ATOM	129	CA	ASN	331	70.311	19.838	65.274	1.00	40.00
ATOM	130	C	ASN	331	70.292	21.336	65.372	1.00	40.00
ATOM	131	O	ASN	331	70.402	21.883	66.467	1.00	40.00
ATOM	132	CB	ASN	331	71.860	19.469	65.312	1.00	40.00
ATOM	133	CG	ASN	331	71.946	17.950	65.562	1.00	40.00
ATOM	134	OD1	ASN	331	70.960	17.310	65.920	1.00	40.00
ATOM	135	ND2	ASN	331	73.165	17.376	65.382	1.00	40.00
ATOM	136	N	ILE	332	70.092	22.047	64.242	1.00	40.00
ATOM	137	CA	ILE	332	70.108	23.485	64.191	1.00	40.00
ATOM	138	C	ILE	332	69.051	24.037	65.100	1.00	40.00
ATOM	139	O	ILE	332	69.149	25.179	65.541	1.00	40.00
ATOM	140	CB	ILE	332	69.769	24.053	62.864	1.00	40.00
ATOM	141	CG1	ILE	332	68.266	23.885	62.540	1.00	40.00
ATOM	142	CG2	ILE	332	70.704	23.413	61.806	1.00	40.00
ATOM	143	CD1	ILE	332	67.726	22.463	62.660	1.00	40.00
ATOM	144	N	LYS	333	67.992	23.281	65.363	1.00	40.00
ATOM	145	CA	LYS	333	66.837	23.647	66.124	1.00	40.00
ATOM	146	C	LYS	333	67.199	24.000	67.537	1.00	40.00
ATOM	147	O	LYS	333	66.528	24.820	68.160	1.00	40.00
ATOM	148	CB	LYS	333	65.769	22.542	66.172	1.00	40.00
ATOM	149	CG	LYS	333	65.218	22.199	64.787	1.00	40.00
ATOM	150	CD	LYS	333	64.406	20.905	64.744	1.00	40.00
ATOM	151	CE	LYS	333	63.906	20.545	63.344	1.00	40.00
ATOM	152	NZ	LYS	333	63.016	21.610	62.832	1.00	40.00
ATOM	153	N	HIS	334	68.273	23.406	68.084	1.00	40.00
ATOM	154	CA	HIS	334	68.644	23.624	69.456	1.00	40.00
ATOM	155	C	HIS	334	68.796	25.099	69.680	1.00	40.00
ATOM	156	O	HIS	334	68.549	25.598	70.776	1.00	40.00
ATOM	157	CB	HIS	334	69.985	22.955	69.807	1.00	40.00
ATOM	158	CG	HIS	334	70.406	23.181	71.234	1.00	40.00
ATOM	159	ND1	HIS	334	69.981	22.368	72.281	1.00	40.00
ATOM	160	CD2	HIS	334	71.250	24.073	71.777	1.00	40.00
ATOM	161	CE1	HIS	334	70.583	22.848	73.400	1.00	40.00
ATOM	162	NE2	HIS	334	71.363	23.882	73.142	1.00	40.00
ATOM	163	N	PHE	335	69.224	25.820	68.629	1.00	40.00
ATOM	164	CA	PHE	335	69.474	27.234	68.584	1.00	40.00
ATOM	165	C	PHE	335	68.254	28.089	68.681	1.00	40.00
ATOM	166	O	PHE	335	68.374	29.298	68.858	1.00	40.00
ATOM	167	CB	PHE	335	70.297	27.691	67.370	1.00	40.00
ATOM	168	CG	PHE	335	71.706	27.589	67.820	1.00	40.00
ATOM	169	CD1	PHE	335	72.240	28.629	68.545	1.00	40.00
ATOM	170	CD2	PHE	335	72.483	26.488	67.544	1.00	40.00
ATOM	171	CE1	PHE	335	73.535	28.586	68.995	1.00	40.00
ATOM	172	CE2	PHE	335	73.781	26.440	67.991	1.00	40.00
ATOM	173	CZ	PHE	335	74.304	27.487	68.715	1.00	40.00
ATOM	174	N	LYS	336	67.051	27.522	68.531	1.00	40.00
ATOM	175	CA	LYS	336	65.866	28.233	68.497	1.00	40.00
ATOM	176	C	LYS	336	65.769	29.252	69.580	1.00	40.00
ATOM	177	O	LYS	336	65.379	30.408	69.520	1.00	40.00
ATOM	178	CB	LYS	336	64.598	27.464	68.435	1.00	40.00
ATOM	179	CG	LYS	336	64.487	26.491	69.611	1.00	40.00
ATOM	180	CD	LYS	336	63.202	25.662	69.617	1.00	40.00
ATOM	181	CE	LYS	336	61.952	26.448	70.013	1.00	40.00
ATOM	182	NZ	LYS	336	60.772	25.556	69.986	1.00	40.00
ATOM	183	N	ASN	337	66.049	28.781	70.909	1.00	40.00
ATOM	184	CA	ASN	337	65.885	29.587	72.098	1.00	40.00
ATOM	185	C	ASN	337	66.954	30.630	72.351	1.00	40.00
ATOM	186	O	ASN	337	66.645	31.726	72.818	1.00	40.00
ATOM	187	CB	ASN	337	65.786	28.723	73.367	1.00	40.00
ATOM	188	CG	ASN	337	64.491	27.932	73.266	1.00	40.00
ATOM	189	OD1	ASN	337	63.580	28.306	72.528	1.00	40.00
ATOM	190	ND2	ASN	337	64.399	26.811	74.031	1.00	40.00

Figure 6 (continued)

ATOM	191	N	CYS	338	68.234	30.326	72.051	1.00	20.00
ATOM	192	CA	CYS	338	69.379	31.056	72.480	1.00	20.00
ATOM	193	C	CYS	338	69.420	32.509	71.971	1.00	20.00
ATOM	194	O	CYS	338	69.349	32.762	70.769	1.00	20.00
ATOM	195	CB	CYS	338	70.719	30.436	72.074	1.00	20.00
ATOM	196	SG	CYS	338	70.738	28.635	72.353	1.00	20.00
ATOM	197	N	THR	339	69.443	33.478	72.915	1.00	20.00
ATOM	198	CA	THR	339	69.718	34.859	72.633	1.00	20.00
ATOM	199	C	THR	339	71.701	35.045	72.625	1.00	20.00
ATOM	200	O	THR	339	71.760	35.739	71.778	1.00	20.00
ATOM	201	CB	THR	339	69.148	35.778	73.671	1.00	20.00
ATOM	202	OG1	THR	339	69.710	35.492	74.943	1.00	20.00
ATOM	203	CG2	THR	339	67.622	35.583	73.710	1.00	20.00
ATOM	204	N	SER	340	71.899	34.433	73.604	1.00	20.00
ATOM	205	CA	SER	340	73.322	34.600	73.667	1.00	20.00
ATOM	206	C	SER	340	73.943	33.319	74.101	1.00	20.00
ATOM	207	O	SER	340	73.883	32.957	75.275	1.00	20.00
ATOM	208	CB	SER	340	73.760	35.676	74.671	1.00	20.00
ATOM	209	OG	SER	340	75.174	35.789	74.682	1.00	20.00
ATOM	210	N	ILE	341	74.599	32.602	73.174	1.00	20.00
ATOM	211	CA	ILE	341	75.211	31.387	73.606	1.00	20.00
ATOM	212	C	ILE	341	76.462	31.743	74.326	1.00	20.00
ATOM	213	O	ILE	341	77.368	32.347	73.758	1.00	20.00
ATOM	214	CB	ILE	341	75.562	30.414	72.516	1.00	20.00
ATOM	215	CG1	ILE	341	76.509	31.042	71.490	1.00	20.00
ATOM	216	CG2	ILE	341	74.273	29.845	71.926	1.00	20.00
ATOM	217	CD1	ILE	341	77.067	30.019	70.499	1.00	20.00
ATOM	218	N	SER	342	76.524	31.398	75.626	1.00	20.00
ATOM	219	CA	SER	342	77.714	31.658	76.372	1.00	20.00
ATOM	220	C	SER	342	78.618	30.489	76.153	1.00	20.00
ATOM	221	O	SER	342	78.595	29.507	76.896	1.00	20.00
ATOM	222	CB	SER	342	77.474	31.836	77.885	1.00	20.00
ATOM	223	OG	SER	342	76.898	30.667	78.447	1.00	20.00
ATOM	224	N	GLY	343	79.443	30.578	75.098	1.00	20.00
ATOM	225	CA	GLY	343	80.341	29.520	74.757	1.00	20.00
ATOM	226	C	GLY	343	80.684	29.709	73.312	1.00	20.00
ATOM	227	O	GLY	343	80.673	30.832	72.814	1.00	20.00
ATOM	228	N	ASP	344	80.915	28.606	72.589	1.00	20.00
ATOM	229	CA	ASP	344	81.297	28.744	71.201	1.00	20.00
ATOM	230	C	ASP	344	80.220	27.989	70.417	1.00	20.00
ATOM	231	O	ASP	344	79.543	27.108	70.942	1.00	20.00
ATOM	232	CB	ASP	344	82.618	28.172	70.836	1.00	20.00
ATOM	233	CG	ASP	344	83.680	29.048	71.486	1.00	20.00
ATOM	234	OD1	ASP	344	83.453	30.284	71.582	1.00	20.00
ATOM	235	OD2	ASP	344	84.728	28.491	71.907	1.00	20.00
ATOM	236	N	LEU	345	80.060	28.353	69.130	1.00	20.00
ATOM	237	CA	LEU	345	79.138	27.650	68.291	1.00	20.00
ATOM	238	C	LEU	345	79.914	27.012	67.189	1.00	20.00
ATOM	239	O	LEU	345b	80.743	27.650	66.546	1.00	20.00
ATOM	240	CB	LEU	345	78.064	28.545	67.655	1.00	20.00
ATOM	241	CG	LEU	345	77.216	27.798	66.613	1.00	20.00
ATOM	242	CD1	LEU	345	76.625	26.510	67.202	1.00	20.00
ATOM	243	CD2	LEU	345	76.147	28.719	66.005	1.00	20.00
ATOM	244	N	HIS	346	79.679	25.705	66.964	1.00	20.00
ATOM	245	CA	HIS	346	80.368	25.032	65.906	1.00	20.00
ATOM	246	C	HIS	346	79.332	24.417	65.028	1.00	20.00
ATOM	247	O	HIS	346	78.422	23.742	65.505	1.00	20.00
ATOM	248	CB	HIS	346	81.271	23.880	66.379	1.00	20.00
ATOM	249	CG	HIS	346	82.367	24.324	67.299	1.00	20.00
ATOM	250	ND1	HIS	346	82.427	24.010	68.639	1.00	20.00
ATOM	251	CD2	HIS	346	83.468	25.083	67.046	1.00	20.00
ATOM	252	CE1	HIS	346	83.553	24.588	69.126	1.00	20.00
ATOM	253	NE2	HIS	346	84.218	25.249	68.197	1.00	20.00
ATOM	254	N	ILE	347	79.422	24.663	63.709	1.00	20.00
ATOM	255	CA	ILE	347	78.486	24.019	62.842	1.00	20.00
ATOM	256	C	ILE	347	79.288	23.208	61.878	1.00	20.00
ATOM	257	O	ILE	347	79.766	23.709	60.861	1.00	20.00
ATOM	258	CB	ILE	347	77.616	24.986	62.092	1.00	20.00
ATOM	259	CG1	ILE	347	76.777	25.795	63.099	1.00	20.00
ATOM	260	CG2	ILE	347	76.768	24.202	61.078	1.00	20.00
ATOM	261	CD1	ILE	347	76.006	26.959	62.479	1.00	20.00
ATOM	262	N	LEU	348	79.435	21.906	62.181	1.00	20.00
ATOM	263	CA	LEU	348	80.215	21.016	61.373	1.00	20.00
ATOM	264	C	LEU	348	79.431	20.711	60.144	1.00	20.00
ATOM	265	O	LEU	348	78.298	21.163	59.978	1.00	20.00
ATOM	266	CB	LEU	348	80.538	19.677	62.066	1.00	20.00
ATOM	267	CG	LEU	348	81.462	19.807	63.290	1.00	20.00

Figure 6 (continued)

ATOM	268	CD1	LEU	348	80.781	20.573	64.436	1.00	20.00
ATOM	269	CD2	LEU	348	81.998	18.435	63.728	1.00	20.00
ATOM	270	N	PRO	349	80.019	19.931	59.216	1.00	20.00
ATOM	271	CA	PRO	349	79.366	19.644	58.037	1.00	20.00
ATOM	272	C	PRO	349	78.014	19.067	58.219	1.00	20.00
ATOM	273	O	PRO	349	77.685	17.991	58.798	1.00	20.00
ATOM	274	CB	PRO	349	80.352	18.799	57.240	1.00	20.00
ATOM	275	CG	PRO	349	81.723	19.295	57.748	1.00	20.00
ATOM	276	CD	PRO	349	81.455	19.787	59.184	1.00	20.00
ATOM	277	N	VAL	350	76.993	19.786	57.726	1.00	40.00
ATOM	278	CA	VAL	350	75.647	19.318	57.787	1.00	40.00
ATOM	279	C	VAL	350	75.029	19.699	56.487	1.00	40.00
ATOM	280	O	VAL	350	75.424	20.690	55.873	1.00	40.00
ATOM	281	CB	VAL	350	74.835	19.957	58.874	1.00	40.00
ATOM	282	CG1	VAL	350	73.395	19.422	58.788	1.00	40.00
ATOM	283	CG2	VAL	350	75.520	19.681	60.223	1.00	40.00
ATOM	284	N	ALA	351	74.046	18.887	56.054	1.00	40.00
ATOM	285	CA	ALA	351	73.308	19.114	54.850	1.00	40.00
ATOM	286	C	ALA	351	71.882	18.863	55.211	1.00	40.00
ATOM	287	O	ALA	351	71.592	18.324	56.270	1.00	40.00
ATOM	288	CB	ALA	351	73.670	18.147	53.711	1.00	40.00
ATOM	289	N	PHE	352	70.942	19.266	54.337	1.00	60.00
ATOM	290	CA	PHE	352	69.562	19.052	54.655	1.00	60.00
ATOM	291	C	PHE	352	69.115	17.830	53.923	1.00	60.00
ATOM	292	O	PHE	352	69.436	17.639	52.752	1.00	60.00
ATOM	293	CB	PHE	352	68.644	20.213	54.235	1.00	60.00
ATOM	294	CG	PHE	352	68.734	20.536	52.754	1.00	60.00
ATOM	295	CD1	PHE	352	69.765	21.037	52.174	1.00	60.00
ATOM	296	CD2	PHE	352	67.787	19.750	51.945	1.00	60.00
ATOM	297	CE1	PHE	352	69.852	21.153	50.807	1.00	60.00
ATOM	298	CE2	PHE	352	67.869	19.863	50.578	1.00	60.00
ATOM	299	CZ	PHE	352	68.903	20.586	50.006	1.00	60.00
ATOM	300	N	ARG	353	68.370	16.994	54.623	1.00	60.00
ATOM	301	CA	ARG	353	67.910	15.761	54.018	1.00	60.00
ATOM	302	C	ARG	353	66.481	15.567	54.413	1.00	60.00
ATOM	303	O	ARG	353	65.982	16.254	55.303	1.00	60.00
ATOM	304	CB	ARG	353	68.631	14.488	54.539	1.00	60.00
ATOM	305	CG	ARG	353	68.391	14.268	56.034	1.00	60.00
ATOM	306	CD	ARG	353	69.082	13.034	56.616	1.00	60.00
ATOM	307	NE	ARG	353	69.733	12.984	58.065	1.00	60.00
ATOM	308	CZ	ARG	353	69.009	11.868	58.801	1.00	60.00
ATOM	309	NH1	ARG	353	69.624	10.799	58.217	1.00	60.00
ATOM	310	NH2	ARG	353	68.671	11.823	60.123	1.00	60.00
ATOM	311	N	GLY	354	65.781	14.634	53.741	1.00	60.00
ATOM	312	CA	GLY	354	64.425	14.346	54.097	1.00	60.00
ATOM	313	C	GLY	354	63.538	15.391	53.511	1.00	60.00
ATOM	314	O	GLY	354	62.364	15.484	53.867	1.00	60.00
ATOM	315	N	ASP	355	64.073	16.214	52.592	1.00	60.00
ATOM	316	CA	ASP	355	63.241	17.225	52.017	1.00	60.00
ATOM	317	C	ASP	355	62.771	16.715	50.698	1.00	60.00
ATOM	318	O	ASP	355	63.557	16.218	49.893	1.00	60.00
ATOM	319	CB	ASP	355	63.970	18.556	51.761	1.00	60.00
ATOM	320	CG	ASP	355	64.250	19.201	53.110	1.00	60.00
ATOM	321	OD1	ASP	355	63.577	18.815	54.103	1.00	60.00
ATOM	322	OD2	ASP	355	65.141	20.089	53.166	1.00	60.00
ATOM	323	N	SER	356	61.451	16.815	50.456	1.00	60.00
ATOM	324	CA	SER	356	60.917	16.363	49.208	1.00	60.00
ATOM	325	C	SER	356	61.282	17.388	48.192	1.00	60.00
ATOM	326	O	SER	356	61.483	18.558	48.518	1.00	60.00
ATOM	327	CB	SER	356	59.387	16.213	49.205	1.00	60.00
ATOM	328	OG	SER	356	58.771	17.476	49.400	1.00	60.00
ATOM	329	N	PHE	357	61.399	16.964	46.921	1.00	60.00
ATOM	330	CA	PHE	357	61.770	17.890	45.898	1.00	60.00
ATOM	331	C	PHE	357	60.708	18.934	45.814	1.00	60.00
ATOM	332	O	PHE	357	61.003	20.127	45.781	1.00	60.00
ATOM	333	CB	PHE	357	61.884	17.240	44.509	1.00	60.00
ATOM	334	CG	PHE	357	63.068	16.333	44.530	1.00	60.00
ATOM	335	CD1	PHE	357	64.329	16.834	44.306	1.00	60.00
ATOM	336	CD2	PHE	357	62.917	14.987	44.771	1.00	60.00
ATOM	337	CE1	PHE	357	65.426	16.005	44.322	1.00	60.00
ATOM	338	CE2	PHE	357	64.010	14.154	44.789	1.00	60.00
ATOM	339	CZ	PHE	357	65.267	14.662	44.564	1.00	60.00
ATOM	340	N	THR	358	59.431	18.510	45.796	1.00	60.00
ATOM	341	CA	THR	358	58.392	19.485	45.675	1.00	60.00
ATOM	342	C	THR	358	57.591	19.530	46.939	1.00	60.00
ATOM	343	O	THR	358	57.220	18.487	47.469	1.00	60.00
ATOM	344	CB	THR	358	57.446	19.217	44.540	1.00	60.00

Figure 6 (continued)

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ATOM   345  OG1 THR   358      56.551  20.308  44.379  1.00 60.00
ATOM   346  CG2 THR   358      56.666  17.953  44.833  1.00 60.00
ATOM   347  N   HIS   359      57.329  20.716  47.445  1.00 60.00
ATOM   348  CA  HIS   359      56.531  20.884  48.621  1.00 60.00
ATOM   349  C   HIS   359      56.047  22.295  48.561  1.00 60.00
ATOM   350  O   HIS   359      56.372  23.027  47.623  1.00 60.00
ATOM   351  CB  HIS   359      57.315  20.697  49.933  1.00 60.00
ATOM   352  CG  HIS   359      56.429  20.549  51.136  1.00 60.00
ATOM   353  ND1 HIS   359      55.994  21.590  51.926  1.00 60.00
ATOM   354  CD2 HIS   359      55.890  19.423  51.680  1.00 60.00
ATOM   355  CE1 HIS   359      55.222  21.046  52.899  1.00 60.00
ATOM   356  NE2 HIS   359      55.129  19.734  52.791  1.00 60.00
ATOM   357  N   THR   360      55.236  22.726  49.547  1.00 60.00
ATOM   358  CA  THR   360      54.780  24.083  49.509  1.00 60.00
ATOM   359  C   THR   360      55.676  24.869  50.406  1.00 60.00
ATOM   360  O   THR   360      55.799  24.563  51.597  1.00 60.00
ATOM   361  CB  THR   360      53.376  24.261  50.010  1.00 60.00
ATOM   362  OG1 THR   360      52.473  23.458  49.224  1.00 60.00
ATOM   363  CG2 THR   360      53.014  25.704  49.934  1.00 60.00
ATOM   364  N   PRO   361      56.334  25.840  49.840  1.00 60.00
ATOM   365  CA  PRO   361      57.221  26.630  50.645  1.00 60.00
ATOM   366  C   PRO   361      56.479  27.590  51.514  1.00 60.00
ATOM   367  O   PRO   361      55.427  28.084  51.114  1.00 60.00
ATOM   368  CB  PRO   361      58.183  27.317  49.673  1.00 60.00
ATOM   369  CG  PRO   361      58.206  26.351  48.472  1.00 60.00
ATOM   370  CD  PRO   361      56.846  25.673  48.486  1.00 60.00
ATOM   371  N   PRO   362      56.999  27.827  52.683  1.00 60.00
ATOM   372  CA  PRO   362      56.413  28.806  53.549  1.00 60.00
ATOM   373  C   PRO   362      56.920  30.135  53.099  1.00 60.00
ATOM   374  O   PRO   362      57.846  30.166  52.290  1.00 60.00
ATOM   375  CB  PRO   362      56.860  28.432  54.965  1.00 60.00
ATOM   376  CG  PRO   362      57.141  26.943  54.894  1.00 60.00
ATOM   377  CD  PRO   362      57.562  26.711  53.436  1.00 60.00
ATOM   378  N   LEU   363      56.338  31.243  53.595  1.00 60.00
ATOM   379  CA  LEU   363      56.852  32.514  53.187  1.00 60.00
ATOM   380  C   LEU   363      58.279  32.631  53.615  1.00 60.00
ATOM   381  O   LEU   363      59.170  32.867  52.835  1.00 60.00
ATOM   382  CB  LEU   363      56.147  33.699  53.871  1.00 60.00
ATOM   383  CG  LEU   363      54.671  33.865  53.464  1.00 60.00
ATOM   384  CD1 LEU   363      54.541  34.253  51.983  1.00 60.00
ATOM   385  CD2 LEU   363      53.845  32.621  53.830  1.00 60.00
ATOM   386  N   ASP   364      58.535  32.141  54.878  1.00 60.00
ATOM   387  CA  ASP   364      59.884  32.075  55.347  1.00 60.00
ATOM   388  C   ASP   364      60.034  30.739  55.998  1.00 60.00
ATOM   389  O   ASP   364      59.242  30.367  56.862  1.00 60.00
ATOM   390  CB  ASP   364      60.220  33.144  56.398  1.00 60.00
ATOM   391  CG  ASP   364      61.724  33.315  56.629  1.00 60.00
ATOM   392  OD1 ASP   364      62.382  32.172  56.114  1.00 60.00
ATOM   393  OD2 ASP   364      62.234  34.038  57.317  1.00 60.00
ATOM   394  N   PRO   365      61.018  29.993  55.587  1.00 60.00
ATOM   395  CA  PRO   365      61.183  28.703  56.196  1.00 60.00
ATOM   396  C   PRO   365      61.803  28.818  57.548  1.00 60.00
ATOM   397  O   PRO   365      62.597  29.730  57.772  1.00 60.00
ATOM   398  CB  PRO   365      61.980  27.861  55.207  1.00 60.00
ATOM   399  CG  PRO   365      61.649  28.494  53.844  1.00 60.00
ATOM   400  CD  PRO   365      61.360  29.968  54.173  1.00 60.00
ATOM   401  N   GLN   366      61.429  27.908  58.467  1.00 60.00
ATOM   402  CA  GLN   366      61.933  27.893  59.809  1.00 60.00
ATOM   403  C   GLN   366      63.377  27.500  59.802  1.00 60.00
ATOM   404  O   GLN   366      64.192  28.068  60.527  1.00 60.00
ATOM   405  CB  GLN   366      61.201  26.866  60.691  1.00 60.00
ATOM   406  CG  GLN   366      59.715  27.169  60.889  1.00 60.00
ATOM   407  CD  GLN   366      59.598  28.345  61.848  1.00 60.00
ATOM   408  OE1 GLN   366      60.197  29.401  61.635  1.00 60.00
ATOM   409  NE2 GLN   366      58.814  28.154  62.942  1.00 60.00
ATOM   410  N   GLU   367      63.724  26.506  58.965  1.00 60.00
ATOM   411  CA  GLU   367      65.044  25.946  58.944  1.00 60.00
ATOM   412  C   GLU   367      66.047  26.988  58.576  1.00 60.00
ATOM   413  O   GLU   367      67.143  27.027  59.132  1.00 60.00
ATOM   414  CB  GLU   367      65.193  24.808  57.921  1.00 60.00
ATOM   415  CG  GLU   367      66.599  24.204  57.891  1.00 60.00
ATOM   416  CD  GLU   367      66.623  23.098  56.846  1.00 60.00
ATOM   417  OE1 GLU   367      65.554  22.842  56.230  1.00 60.00
ATOM   418  OE2 GLU   367      67.711  22.497  56.648  1.00 60.00
ATOM   419  N   LEU   368      65.692  27.870  57.631  1.00 40.00
ATOM   420  CA  LEU   368      66.639  28.826  57.149  1.00 40.00
ATOM   421  C   LEU   368      67.144  29.693  58.252  1.00 40.00
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Figure 6 (continued)

ATOM	422	O	LEU	368	68.335	29.999	58.285	1.00	40.00
ATOM	423	CB	LEU	368	66.064	29.752	56.062	1.00	40.00
ATOM	424	CG	LEU	368	65.883	29.062	54.695	1.00	40.00
ATOM	425	CD1	LEU	368	64.978	27.828	54.805	1.00	40.00
ATOM	426	CD2	LEU	368	65.403	30.061	53.635	1.00	40.00
ATOM	427	N	ASP	369	66.285	30.128	59.191	1.00	40.00
ATOM	428	CA	ASP	369	66.841	31.074	60.102	1.00	40.00
ATOM	429	C	ASP	369	66.613	30.516	61.451	1.00	40.00
ATOM	430	O	ASP	369	65.469	30.262	61.829	1.00	40.00
ATOM	431	CB	ASP	369	66.170	32.458	60.047	1.00	40.00
ATOM	432	CG	ASP	369	66.548	33.104	58.722	1.00	40.00
ATOM	433	OD1	ASP	369	67.460	32.565	58.041	1.00	40.00
ATOM	434	OD2	ASP	369	65.930	34.146	58.375	1.00	40.00
ATOM	435	N	ILE	370	67.712	30.280	62.196	1.00	40.00
ATOM	436	CA	ILE	370	67.553	29.772	63.520	1.00	40.00
ATOM	437	C	ILE	370	66.701	30.773	64.204	1.00	40.00
ATOM	438	O	ILE	370	65.566	30.470	64.562	1.00	40.00
ATOM	439	CB	ILE	370	68.847	29.669	64.271	1.00	40.00
ATOM	440	CG1	ILE	370	69.762	28.617	63.621	1.00	40.00
ATOM	441	CG2	ILE	370	68.511	29.380	65.741	1.00	40.00
ATOM	442	CD1	ILE	370	70.227	28.988	62.213	1.00	40.00
ATOM	443	N	LEU	371	67.219	32.008	64.350	1.00	40.00
ATOM	444	CA	LEU	371	66.429	33.061	64.908	1.00	40.00
ATOM	445	C	LEU	371	67.159	34.349	64.879	1.00	40.00
ATOM	446	O	LEU	371	68.388	34.417	64.889	1.00	40.00
ATOM	447	CB	LEU	371	65.945	32.913	66.367	1.00	40.00
ATOM	448	CG	LEU	371	64.669	32.077	66.572	1.00	40.00
ATOM	449	CD1	LEU	371	64.092	32.270	67.981	1.00	40.00
ATOM	450	CD2	LEU	371	63.638	32.356	65.466	1.00	40.00
ATOM	451	N	LYS	372	66.340	35.410	64.862	1.00	40.00
ATOM	452	CA	LYS	372	66.715	36.782	64.924	1.00	40.00
ATOM	453	C	LYS	372	67.209	36.960	66.320	1.00	40.00
ATOM	454	O	LYS	372	67.897	37.934	66.640	1.00	40.00
ATOM	455	CB	LYS	372	65.504	37.709	64.728	1.00	40.00
ATOM	456	CG	LYS	372	64.697	37.378	63.470	1.00	40.00
ATOM	457	CD	LYS	372	65.522	37.345	62.182	1.00	40.00
ATOM	458	CE	LYS	372	64.722	36.862	60.970	1.00	40.00
ATOM	459	NZ	LYS	372	65.633	36.538	59.850	1.00	40.00
ATOM	460	N	THR	373	66.817	36.028	67.196	1.00	20.00
ATOM	461	CA	THR	373	67.096	36.060	68.601	1.00	20.00
ATOM	462	C	THR	373	68.570	36.057	68.880	1.00	20.00
ATOM	463	O	THR	373	68.998	36.664	69.859	1.00	20.00
ATOM	464	CB	THR	373	66.506	34.891	69.335	1.00	20.00
ATOM	465	OG1	THR	373	66.624	35.085	70.737	1.00	20.00
ATOM	466	CG2	THR	373	67.254	33.616	68.912	1.00	20.00
ATOM	467	N	VAL	374	69.395	35.381	68.054	1.00	20.00
ATOM	468	CA	VAL	374	70.787	35.278	68.409	1.00	20.00
ATOM	469	C	VAL	374	71.534	36.552	68.122	1.00	20.00
ATOM	470	O	VAL	374	71.901	36.845	66.984	1.00	20.00
ATOM	471	CB	VAL	374	71.482	34.137	67.722	1.00	20.00
ATOM	472	CG1	VAL	374	70.891	32.822	68.257	1.00	20.00
ATOM	473	CG2	VAL	374	71.308	34.292	66.201	1.00	20.00
ATOM	474	N	LYS	375	71.703	37.377	69.179	1.00	20.00
ATOM	475	CA	LYS	375	72.455	38.601	69.171	1.00	20.00
ATOM	476	C	LYS	375	73.934	38.356	69.276	1.00	20.00
ATOM	477	O	LYS	375	74.724	38.952	68.548	1.00	20.00
ATOM	478	CB	LYS	375	72.104	39.515	70.357	1.00	20.00
ATOM	479	CG	LYS	375	70.652	39.992	70.380	1.00	20.00
ATOM	480	CD	LYS	375	70.253	40.621	71.716	1.00	20.00
ATOM	481	CE	LYS	375	70.283	39.635	72.886	1.00	20.00
ATOM	482	NZ	LYS	375	70.032	40.347	74.158	1.00	20.00
ATOM	483	N	GLU	376	74.370	37.463	70.191	1.00	20.00
ATOM	484	CA	GLU	376	75.790	37.398	70.390	1.00	20.00
ATOM	485	C	GLU	376	76.248	36.006	70.665	1.00	20.00
ATOM	486	O	GLU	376	75.456	35.084	70.842	1.00	20.00
ATOM	487	CB	GLU	376	76.269	38.271	71.562	1.00	20.00
ATOM	488	CG	GLU	376	75.648	37.879	72.903	1.00	20.00
ATOM	489	CD	GLU	376	76.201	38.809	73.974	1.00	20.00
ATOM	490	OE1	GLU	376	77.445	39.001	74.011	1.00	20.00
ATOM	491	OE2	GLU	376	75.380	39.346	74.768	1.00	20.00
ATOM	492	N	ILE	377	77.586	35.845	70.643	1.00	20.00
ATOM	493	CA	ILE	377	78.258	34.675	70.961	1.00	20.00
ATOM	494	C	ILE	377	79.458	35.085	71.726	1.00	20.00
ATOM	495	O	ILE	377	80.208	35.939	71.258	1.00	20.00
ATOM	496	CB	ILE	377	78.729	33.891	69.741	1.00	20.00
ATOM	497	CG1	ILE	377	77.532	33.564	68.831	1.00	20.00
ATOM	498	CG2	ILE	377	79.513	32.649	70.196	1.00	20.00

Figure 6 (continued)

ATOM	499	CD1	ILE	377	77.935	33.085	67.437	1.00 20.00
ATOM	500	N	THR	378	79.661	34.637	72.932	1.00 20.00
ATOM	501	CA	THR	378	80.705	34.958	73.870	1.00 20.00
ATOM	502	C	THR	378	82.055	34.508	73.356	1.00 20.00
ATOM	503	O	THR	378	83.055	34.926	73.931	1.00 20.00
ATOM	504	CB	THR	378	80.542	34.462	75.271	1.00 20.00
ATOM	505	OG1	THR	378	81.409	35.175	76.093	1.00 20.00
ATOM	506	CG2	THR	378	80.913	32.976	75.242	1.00 20.00
ATOM	507	N	GLY	379	82.134	33.568	72.394	1.00 20.00
ATOM	508	CA	GLY	379	83.421	33.057	72.000	1.00 20.00
ATOM	509	C	GLY	379	83.656	33.287	70.540	1.00 20.00
ATOM	510	O	GLY	379	83.795	34.434	70.097	1.00 20.00
ATOM	511	N	PHE	380	83.754	32.204	69.755	1.00 20.00
ATOM	512	CA	PHE	380	83.990	32.339	68.346	1.00 20.00
ATOM	513	C	PHE	380	82.939	31.569	67.615	1.00 20.00
ATOM	514	O	PHE	380	82.209	30.782	68.214	1.00 20.00
ATOM	515	CB	PHE	380	85.380	31.855	67.885	1.00 20.00
ATOM	516	CG	PHE	380	85.531	30.395	68.158	1.00 20.00
ATOM	517	CD1	PHE	380	85.154	29.462	67.218	1.00 20.00
ATOM	518	CD2	PHE	380	86.057	29.961	69.352	1.00 20.00
ATOM	519	CE1	PHE	380	85.298	28.117	67.467	1.00 20.00
ATOM	520	CE2	PHE	380	86.203	28.617	69.604	1.00 20.00
ATOM	521	CZ	PHE	380	85.823	27.693	68.663	1.00 20.00
ATOM	522	N	LEU	381	82.806	31.821	66.294	1.00 20.00
ATOM	523	CA	LEU	381	81.819	31.147	65.497	1.00 20.00
ATOM	524	C	LEU	381	82.535	30.365	64.432	1.00 20.00
ATOM	525	O	LEU	381	83.374	30.913	63.665	1.00 20.00
ATOM	526	CB	LEU	381	80.845	32.133	64.819	1.00 20.00
ATOM	527	CG	LEU	381	79.760	31.407	63.947	1.00 20.00
ATOM	528	CD1	LEU	381	78.861	30.553	64.762	1.00 20.00
ATOM	529	CD2	LEU	381	78.952	32.558	63.189	1.00 20.00
ATOM	530	N	LEU	382	82.277	29.060	64.360	1.00 20.00
ATOM	531	CA	LEU	382	82.974	28.221	63.407	1.00 20.00
ATOM	532	C	LEU	382	81.989	27.496	62.539	1.00 20.00
ATOM	533	O	LEU	382	81.199	26.684	63.018	1.00 20.00
ATOM	534	CB	LEU	382	83.864	27.171	64.102	1.00 20.00
ATOM	535	CG	LEU	382	84.655	26.245	63.164	1.00 20.00
ATOM	536	CD1	LEU	382	85.836	27.027	62.283	1.00 20.00
ATOM	537	CD2	LEU	382	85.343	25.128	63.965	1.00 20.00
ATOM	538	N	ILE	383	82.013	27.781	61.220	1.00 20.00
ATOM	539	CA	ILE	383	81.137	27.094	60.316	1.00 20.00
ATOM	540	C	ILE	383	82.015	26.374	59.368	1.00 20.00
ATOM	541	O	ILE	383	82.648	26.989	58.493	1.00 20.00
ATOM	542	CB	ILE	383	80.282	28.016	59.500	1.00 20.00
ATOM	543	CG1	ILE	383	79.404	28.888	60.409	1.00 20.00
ATOM	544	CG2	ILE	383	79.482	27.156	58.505	1.00 20.00
ATOM	545	CD1	ILE	383	78.460	28.082	61.296	1.00 20.00
ATOM	546	N	GLN	384	82.074	25.038	59.443	1.00 20.00
ATOM	547	CA	GLN	384	82.915	24.339	58.526	1.00 20.00
ATOM	548	C	GLN	384	82.054	23.458	57.685	1.00 20.00
ATOM	549	O	GLN	384	81.117	22.832	58.177	1.00 20.00
ATOM	550	CB	GLN	384	83.961	23.439	59.207	1.00 20.00
ATOM	551	CG	GLN	384	84.855	22.697	58.213	1.00 20.00
ATOM	552	CD	GLN	384	85.837	21.843	59.002	1.00 20.00
ATOM	553	OE1	GLN	384	86.450	22.308	59.961	1.00 20.00
ATOM	554	NE2	GLN	384	85.991	20.556	58.592	1.00 20.00
ATOM	555	N	ALA	385	82.371	23.410	56.375	1.00 20.00
ATOM	556	CA	ALA	385	81.706	22.591	55.398	1.00 20.00
ATOM	557	C	ALA	385	80.224	22.590	55.601	1.00 20.00
ATOM	558	O	ALA	385	79.661	21.620	56.106	1.00 20.00
ATOM	559	CB	ALA	385	82.195	21.134	55.384	1.00 20.00
ATOM	560	N	TRP	386	79.551	23.693	55.231	1.00 40.00
ATOM	561	CA	TRP	386	78.121	23.719	55.326	1.00 40.00
ATOM	562	C	TRP	386	77.603	23.977	53.951	1.00 40.00
ATOM	563	O	TRP	386	77.704	25.086	53.430	1.00 40.00
ATOM	564	CB	TRP	386	77.603	24.843	56.245	1.00 40.00
ATOM	565	CG	TRP	386	76.100	25.012	56.311	1.00 40.00
ATOM	566	CD1	TRP	386	75.140	24.767	55.366	1.00 40.00
ATOM	567	CD2	TRP	386	75.403	25.494	57.469	1.00 40.00
ATOM	568	NE1	TRP	386	73.904	25.079	55.856	1.00 40.00
ATOM	569	CE2	TRP	386	74.046	25.525	57.152	1.00 40.00
ATOM	570	CE3	TRP	386	75.857	25.881	58.698	1.00 40.00
ATOM	571	CZ2	TRP	386	73.118	25.943	58.063	1.00 40.00
ATOM	572	CZ3	TRP	386	74.919	26.302	59.614	1.00 40.00
ATOM	573	CH2	TRP	386	73.575	26.332	59.302	1.00 40.00
ATOM	574	N	PRO	387	77.111	22.950	53.320	1.00 40.00
ATOM	575	CA	PRO	387	76.494	23.101	52.046	1.00 40.00

Figure 6 (continued)

ATOM	576	C	PRO	387	75.105	23.656	52.308	1.00	40.00
ATOM	577	O	PRO	387	74.486	23.158	53.248	1.00	40.00
ATOM	578	CB	PRO	387	76.546	21.853	51.296	1.00	40.00
ATOM	579	CG	PRO	387	77.766	21.143	51.909	1.00	40.00
ATOM	580	CD	PRO	387	77.837	21.690	53.344	1.00	40.00
ATOM	581	N	GLU	388	74.578	24.599	51.507	1.00	60.00
ATOM	582	CA	GLU	388	73.232	25.004	51.769	1.00	60.00
ATOM	583	C	GLU	388	72.859	26.053	50.778	1.00	60.00
ATOM	584	O	GLU	388	73.126	27.236	50.973	1.00	60.00
ATOM	585	CB	GLU	388	73.030	25.606	53.170	1.00	60.00
ATOM	586	CG	GLU	388	71.562	25.867	53.513	1.00	60.00
ATOM	587	CD	GLU	388	70.869	24.625	53.757	1.00	60.00
ATOM	588	OE1	GLU	388	71.564	23.618	54.314	1.00	60.00
ATOM	589	OE2	GLU	388	69.693	24.388	53.386	1.00	60.00
ATOM	590	N	ASN	389	72.239	25.631	49.664	1.00	60.00
ATOM	591	CA	ASN	389	71.795	26.572	48.685	1.00	60.00
ATOM	592	C	ASN	389	70.669	27.338	49.296	1.00	60.00
ATOM	593	O	ASN	389	70.529	28.543	49.090	1.00	60.00
ATOM	594	CB	ASN	389	71.262	25.904	47.407	1.00	60.00
ATOM	595	CG	ASN	389	72.438	26.279	46.670	1.00	60.00
ATOM	596	OD1	ASN	389	73.467	25.921	46.464	1.00	60.00
ATOM	597	ND2	ASN	389	72.287	23.990	46.286	1.00	60.00
ATOM	598	N	ARG	390	69.832	26.632	50.079	1.00	60.00
ATOM	599	CA	ARG	390	68.661	27.215	50.663	1.00	60.00
ATOM	600	C	ARG	390	69.044	28.334	51.576	1.00	60.00
ATOM	601	O	ARG	390	68.487	29.427	51.481	1.00	60.00
ATOM	602	CB	ARG	390	67.659	26.203	51.500	1.00	60.00
ATOM	603	CG	ARG	390	67.276	25.053	50.678	1.00	60.00
ATOM	604	CD	ARG	390	66.479	24.044	51.506	1.00	60.00
ATOM	605	NE	ARG	390	66.180	24.678	51.872	1.00	60.00
ATOM	606	CZ	ARG	390	64.189	23.927	52.437	1.00	60.00
ATOM	607	NH1	ARG	390	64.394	22.599	52.678	1.00	60.00
ATOM	608	NH2	ARG	390	62.995	24.504	52.761	1.00	60.00
ATOM	609	N	THR	391	70.013	28.112	52.482	1.00	60.00
ATOM	610	CA	THR	391	70.321	29.182	53.385	1.00	60.00
ATOM	611	C	THR	391	71.800	29.287	53.543	1.00	60.00
ATOM	612	O	THR	391	72.554	28.398	53.154	1.00	60.00
ATOM	613	CB	THR	391	69.738	29.001	54.755	1.00	60.00
ATOM	614	OG1	THR	391	69.919	30.181	55.524	1.00	60.00
ATOM	615	CG2	THR	391	70.431	27.808	55.437	1.00	60.00
ATOM	616	N	ASP	392	72.250	30.418	54.118	1.00	60.00
ATOM	617	CA	ASP	392	73.648	30.631	54.330	1.00	60.00
ATOM	618	C	ASP	392	73.787	31.156	55.719	1.00	60.00
ATOM	619	O	ASP	392	73.183	30.646	56.662	1.00	60.00
ATOM	620	CB	ASP	392	74.243	31.706	53.404	1.00	60.00
ATOM	621	CG	ASP	392	74.233	31.177	51.977	1.00	60.00
ATOM	622	OD1	ASP	392	74.198	29.930	51.808	1.00	60.00
ATOM	623	OD2	ASP	392	74.257	32.017	51.038	1.00	60.00
ATOM	624	N	LEU	393	74.606	32.211	55.857	1.00	40.00
ATOM	625	CA	LEU	393	74.836	32.877	57.102	1.00	40.00
ATOM	626	C	LEU	393	73.560	33.562	57.449	1.00	40.00
ATOM	627	O	LEU	393	73.360	33.992	58.584	1.00	40.00
ATOM	628	CB	LEU	393	75.983	33.887	57.086	1.00	40.00
ATOM	629	CG	LEU	393	77.357	33.257	56.797	1.00	40.00
ATOM	630	CD1	LEU	393	77.402	32.639	55.390	1.00	40.00
ATOM	631	CD2	LEU	393	78.494	34.263	57.041	1.00	40.00
ATOM	632	N	HIS	394	72.640	33.649	56.465	1.00	40.00
ATOM	633	CA	HIS	394	71.336	34.221	56.682	1.00	40.00
ATOM	634	C	HIS	394	70.664	33.594	57.865	1.00	40.00
ATOM	635	O	HIS	394	69.672	34.124	58.366	1.00	40.00
ATOM	636	CB	HIS	394	70.393	34.073	55.475	1.00	40.00
ATOM	637	CG	HIS	394	70.691	35.047	54.373	1.00	40.00
ATOM	638	ND1	HIS	394	70.133	36.304	54.296	1.00	40.00
ATOM	639	CD2	HIS	394	71.506	34.935	53.289	1.00	40.00
ATOM	640	CE1	HIS	394	70.635	36.887	53.177	1.00	40.00
ATOM	641	NE2	HIS	394	71.473	36.094	52.534	1.00	40.00
ATOM	642	N	ALA	395	71.156	32.439	58.340	1.00	20.00
ATOM	643	CA	ALA	395	70.541	31.844	59.484	1.00	20.00
ATOM	644	C	ALA	395	70.580	32.834	60.613	1.00	20.00
ATOM	645	O	ALA	395	69.605	32.955	61.356	1.00	20.00
ATOM	646	CB	ALA	395	71.272	30.573	59.954	1.00	20.00
ATOM	647	N	PHE	396	71.698	33.575	60.788	1.00	20.00
ATOM	648	CA	PHE	396	71.740	34.491	61.898	1.00	20.00
ATOM	649	C	PHE	396	71.749	35.899	61.382	1.00	20.00
ATOM	650	O	PHE	396	72.809	36.531	61.312	1.00	20.00
ATOM	651	CB	PHE	396	73.029	34.358	62.727	1.00	20.00
ATOM	652	CG	PHE	396	73.183	32.935	63.142	1.00	20.00

Figure 6 (continued)

ATOM	653	CD1	PHE	396	72.612	32.480	64.300	1.00	20.00
ATOM	654	CD2	PHE	396	73.905	32.065	62.356	1.00	20.00
ATOM	655	CE1	PHE	396	72.762	31.145	64.670	1.00	20.00
ATOM	656	CE2	PHE	396	74.060	30.741	62.720	1.00	20.00
ATOM	657	CZ	PHE	396	73.487	30.285	63.681	1.00	20.00
ATOM	658	N	GLU	397	70.573	36.462	61.049	1.00	20.00
ATOM	659	CA	GLU	397	70.594	37.795	60.518	1.00	20.00
ATOM	660	C	GLU	397	70.975	38.784	61.582	1.00	20.00
ATOM	661	O	GLU	397	71.603	39.794	61.287	1.00	20.00
ATOM	662	CB	GLU	397	69.278	38.264	59.887	1.00	20.00
ATOM	663	CG	GLU	397	68.147	38.517	60.877	1.00	20.00
ATOM	664	CD	GLU	397	67.181	39.513	60.218	1.00	20.00
ATOM	665	OE1	GLU	397	66.395	39.079	59.337	1.00	20.00
ATOM	666	OE2	GLU	397	67.230	40.716	60.587	1.00	20.00
ATOM	667	N	ASN	398	70.564	38.545	62.837	1.00	20.00
ATOM	668	CA	ASN	398	70.744	39.439	63.953	1.00	20.00
ATOM	669	C	ASN	398	72.098	39.431	64.607	1.00	20.00
ATOM	670	O	ASN	398	72.390	40.373	65.344	1.00	20.00
ATOM	671	CB	ASN	398	69.706	39.249	65.061	1.00	20.00
ATOM	672	CG	ASN	398	68.421	39.874	64.550	1.00	20.00
ATOM	673	OD1	ASN	398	68.058	40.988	64.927	1.00	20.00
ATOM	674	ND2	ASN	398	67.725	39.151	63.637	1.00	20.00
ATOM	675	N	LEU	399	72.927	38.382	64.425	1.00	20.00
ATOM	676	CA	LEU	399	74.176	38.231	65.142	1.00	20.00
ATOM	677	C	LEU	399	74.964	39.516	65.126	1.00	20.00
ATOM	678	O	LEU	399	75.513	39.904	64.095	1.00	20.00
ATOM	679	CB	LEU	399	75.056	37.121	64.540	1.00	20.00
ATOM	680	CG	LEU	399	76.401	36.912	65.257	1.00	20.00
ATOM	681	CD1	LEU	399	76.193	36.416	66.702	1.00	20.00
ATOM	682	CD2	LEU	399	77.320	35.989	64.438	1.00	20.00
ATOM	683	N	GLU	400	74.935	40.242	66.273	1.00	20.00
ATOM	684	CA	GLU	400	75.597	41.501	66.503	1.00	20.00
ATOM	685	C	GLU	400	77.060	41.434	66.883	1.00	20.00
ATOM	686	O	GLU	400	77.869	42.168	66.319	1.00	20.00
ATOM	687	CB	GLU	400	74.861	42.348	67.559	1.00	20.00
ATOM	688	CG	GLU	400	74.722	41.671	68.923	1.00	20.00
ATOM	689	CD	GLU	400	73.765	42.509	69.759	1.00	20.00
ATOM	690	OE1	GLU	400	72.878	43.169	69.156	1.00	20.00
ATOM	691	OE2	GLU	400	73.906	42.499	71.011	1.00	20.00
ATOM	692	N	ILE	401	77.466	40.569	67.842	1.00	20.00
ATOM	693	CA	ILE	401	78.841	40.653	68.276	1.00	20.00
ATOM	694	C	ILE	401	79.358	39.294	68.644	1.00	20.00
ATOM	695	O	ILE	401	78.608	38.434	69.104	1.00	20.00
ATOM	696	CB	ILE	401	79.008	41.515	69.498	1.00	20.00
ATOM	697	CG1	ILE	401	78.513	42.966	69.227	1.00	20.00
ATOM	698	CG2	ILE	401	80.479	41.456	69.940	1.00	20.00
ATOM	699	CD1	ILE	401	78.378	43.788	70.495	1.00	20.00
ATOM	700	N	ILE	402	80.677	39.078	68.431	1.00	20.00
ATOM	701	CA	ILE	402	81.346	37.859	68.793	1.00	20.00
ATOM	702	C	ILE	402	82.483	38.282	69.677	1.00	20.00
ATOM	703	O	ILE	402	83.526	38.710	69.195	1.00	20.00
ATOM	704	CB	ILE	402	81.934	37.164	67.596	1.00	20.00
ATOM	705	CG1	ILE	402	80.828	36.793	66.594	1.00	20.00
ATOM	706	CG2	ILE	402	82.752	35.959	68.080	1.00	20.00
ATOM	707	CD1	ILE	402	81.361	36.376	65.225	1.00	20.00
ATOM	708	N	ARG	403	82.340	38.091	71.000	1.00	20.00
ATOM	709	CA	ARG	403	83.249	38.630	71.978	1.00	20.00
ATOM	710	C	ARG	403	84.656	38.156	71.775	1.00	20.00
ATOM	711	O	ARG	403	85.595	38.916	72.000	1.00	20.00
ATOM	712	CB	ARG	403	82.835	38.270	73.414	1.00	20.00
ATOM	713	CG	ARG	403	81.404	38.709	73.735	1.00	20.00
ATOM	714	CD	ARG	403	81.024	38.588	75.212	1.00	20.00
ATOM	715	NE	ARG	403	80.986	39.968	75.776	1.00	20.00
ATOM	716	CZ	ARG	403	82.100	40.523	76.334	1.00	20.00
ATOM	717	NH1	ARG	403	83.264	39.812	76.393	1.00	20.00
ATOM	718	NH2	ARG	403	82.049	41.791	76.836	1.00	20.00
ATOM	719	N	GLY	404	84.866	36.889	71.303	1.00	20.00
ATOM	720	CA	GLY	404	86.209	36.427	71.177	1.00	20.00
ATOM	721	C	GLY	404	86.879	36.183	72.495	1.00	20.00
ATOM	722	O	GLY	404	88.106	36.208	72.584	1.00	20.00
ATOM	723	N	ARG	405	86.099	35.916	73.559	1.00	20.00
ATOM	724	CA	ARG	405	86.700	35.672	74.839	1.00	20.00
ATOM	725	C	ARG	405	87.611	34.502	74.670	1.00	20.00
ATOM	726	O	ARG	405	88.728	34.489	75.184	1.00	20.00
ATOM	727	CB	ARG	405	85.674	35.303	75.925	1.00	20.00
ATOM	728	CG	ARG	405	84.794	36.474	76.364	1.00	20.00
ATOM	729	CD	ARG	405	85.274	37.144	77.654	1.00	20.00

Figure 6 (continued)

ATOM	730	NE	ARG	405	86.553	37.843	77.350	1.00	20.00
ATOM	731	CZ	ARG	405	87.191	38.551	78.326	1.00	20.00
ATOM	732	NH1	ARG	405	86.659	38.613	79.582	1.00	20.00
ATOM	733	NH2	ARG	405	88.362	39.196	78.049	1.00	20.00
ATOM	734	N	THR	406	87.144	33.483	73.930	1.00	20.00
ATOM	735	CA	THR	406	87.965	32.345	73.649	1.00	20.00
ATOM	736	C	THR	406	88.001	32.248	72.162	1.00	20.00
ATOM	737	O	THR	406	86.972	32.378	71.504	1.00	20.00
ATOM	738	CB	THR	406	87.398	31.084	74.180	1.00	20.00
ATOM	739	OG1	THR	406	87.233	31.114	75.569	1.00	20.00
ATOM	740	CG2	THR	406	88.359	29.913	73.786	1.00	20.00
ATOM	741	N	LYS	407	89.193	32.019	71.586	1.00	20.00
ATOM	742	CA	LYS	407	89.281	31.979	70.157	1.00	20.00
ATOM	743	C	LYS	407	89.797	30.645	69.747	1.00	20.00
ATOM	744	O	LYS	407	90.399	29.926	70.543	1.00	20.00
ATOM	745	CB	LYS	407	90.238	33.037	69.681	1.00	20.00
ATOM	746	CG	LYS	407	91.679	32.884	70.077	1.00	20.00
ATOM	747	CD	LYS	407	91.825	33.046	71.593	1.00	20.00
ATOM	748	CE	LYS	407	93.248	32.835	72.110	1.00	20.00
ATOM	749	NZ	LYS	407	93.280	33.013	73.580	1.00	20.00
ATOM	750	N	GLN	408	89.538	30.258	68.481	1.00	20.00
ATOM	751	CA	GLN	408	90.096	29.017	68.051	1.00	20.00
ATOM	752	C	GLN	408	91.483	29.349	67.630	1.00	20.00
ATOM	753	O	GLN	408	91.763	30.501	67.296	1.00	20.00
ATOM	754	CB	GLN	408	89.396	28.341	66.863	1.00	20.00
ATOM	755	CG	GLN	408	89.499	29.103	65.547	1.00	20.00
ATOM	756	CD	GLN	408	89.073	28.124	64.465	1.00	20.00
ATOM	757	OE1	GLN	408	88.607	28.513	63.398	1.00	20.00
ATOM	758	NE2	GLN	408	89.245	26.805	64.747	1.00	20.00
ATOM	759	N	HIS	409	92.375	28.340	67.629	1.00	20.00
ATOM	760	CA	HIS	409	93.764	28.549	67.341	1.00	20.00
ATOM	761	C	HIS	409	93.872	29.295	66.062	1.00	20.00
ATOM	762	O	HIS	409	93.018	29.181	65.186	1.00	20.00
ATOM	763	CB	HIS	409	94.579	27.249	67.237	1.00	20.00
ATOM	764	CG	HIS	409	94.658	26.518	68.547	1.00	20.00
ATOM	765	ND1	HIS	409	93.716	26.612	68.986	1.00	20.00
ATOM	766	CD2	HIS	409	95.598	26.582	69.531	1.00	20.00
ATOM	767	CE1	HIS	409	94.127	25.180	70.204	1.00	20.00
ATOM	768	NE2	HIS	409	95.263	25.739	70.577	1.00	20.00
ATOM	769	N	GLY	410	94.929	30.113	65.945	1.00	20.00
ATOM	770	CA	GLY	410	95.035	30.978	64.915	1.00	20.00
ATOM	771	C	GLY	410	94.356	32.221	65.273	1.00	20.00
ATOM	772	O	GLY	410	94.314	33.233	64.575	1.00	20.00
ATOM	773	N	GLN	411	93.822	32.149	66.508	1.00	20.00
ATOM	774	CA	GLN	411	93.134	33.238	67.131	1.00	20.00
ATOM	775	C	GLN	411	92.065	33.728	66.212	1.00	20.00
ATOM	776	O	GLN	411	92.036	34.909	65.870	1.00	20.00
ATOM	777	CB	GLN	411	94.060	34.410	67.478	1.00	20.00
ATOM	778	CG	GLN	411	95.139	34.061	68.503	1.00	20.00
ATOM	779	CD	GLN	411	95.978	35.307	68.753	1.00	20.00
ATOM	780	OE1	GLN	411	96.291	35.640	69.895	1.00	20.00
ATOM	781	NE2	GLN	411	96.362	36.010	67.656	1.00	20.00
ATOM	782	N	PHE	412	91.150	32.832	65.791	1.00	20.00
ATOM	783	CA	PHE	412	90.107	33.253	64.904	1.00	20.00
ATOM	784	C	PHE	412	88.828	33.358	65.669	1.00	20.00
ATOM	785	O	PHE	412	88.440	32.453	66.404	1.00	20.00
ATOM	786	CB	PHE	412	89.843	32.287	63.737	1.00	20.00
ATOM	787	CG	PHE	412	91.064	32.280	62.885	1.00	20.00
ATOM	788	CD1	PHE	412	91.356	33.347	62.070	1.00	20.00
ATOM	789	CD2	PHE	412	91.911	31.197	62.892	1.00	20.00
ATOM	790	CE1	PHE	412	92.482	33.338	61.279	1.00	20.00
ATOM	791	CE2	PHE	412	93.037	31.184	62.103	1.00	20.00
ATOM	792	CZ	PHE	412	93.326	32.256	61.296	1.00	20.00
ATOM	793	N	SER	413	88.193	34.538	65.566	1.00	20.00
ATOM	794	CA	SER	413	86.914	34.839	66.139	1.00	20.00
ATOM	795	C	SER	413	85.866	34.220	65.282	1.00	20.00
ATOM	796	O	SER	413	84.871	33.694	65.779	1.00	20.00
ATOM	797	CB	SER	413	86.618	36.342	66.092	1.00	20.00
ATOM	798	OG	SER	413	87.743	37.068	66.556	1.00	20.00
ATOM	799	N	LEU	414	86.058	34.318	63.953	1.00	20.00
ATOM	800	CA	LEU	414	85.098	33.828	63.009	1.00	20.00
ATOM	801	C	LEU	414	85.822	33.010	61.998	1.00	20.00
ATOM	802	O	LEU	414	86.615	33.527	61.212	1.00	20.00
ATOM	803	CB	LEU	414	84.395	34.969	62.249	1.00	20.00
ATOM	804	CG	LEU	414	83.351	34.505	61.219	1.00	20.00
ATOM	805	CD1	LEU	414	82.172	33.785	61.890	1.00	20.00
ATOM	806	CD2	LEU	414	82.913	35.673	60.318	1.00	20.00

Figure 6 (continued)

ATOM	807	N	ALA	415	85.568	31.694	61.983	1.00 20.00
ATOM	808	CA	ALA	415	86.220	30.917	60.979	1.00 20.00
ATOM	809	C	ALA	415	85.159	30.337	60.115	1.00 20.00
ATOM	810	O	ALA	415	84.230	29.704	60.610	1.00 20.00
ATOM	811	CB	ALA	415	87.039	29.744	61.526	1.00 20.00
ATOM	812	N	VAL	416	85.251	30.584	58.794	1.00 20.00
ATOM	813	CA	VAL	416	84.332	29.982	57.878	1.00 20.00
ATOM	814	C	VAL	416	85.159	29.237	56.878	1.00 20.00
ATOM	815	O	VAL	416	85.846	25.874	56.045	1.00 20.00
ATOM	816	CB	VAL	416	83.440	30.973	57.174	1.00 20.00
ATOM	817	CG1	VAL	416	82.494	31.577	58.227	1.00 20.00
ATOM	818	CG2	VAL	416	84.296	32.026	56.465	1.00 20.00
ATOM	819	N	VAL	417	85.121	27.894	56.935	1.00 20.00
ATOM	820	CA	VAL	417	85.951	27.162	56.027	1.00 20.00
ATOM	821	C	VAL	417	85.085	26.285	55.183	1.00 20.00
ATOM	822	O	VAL	417	84.125	25.692	55.673	1.00 20.00
ATOM	823	CB	VAL	417	86.949	26.276	56.717	1.00 20.00
ATOM	824	CG1	VAL	417	87.911	27.163	57.525	1.00 20.00
ATOM	825	CG2	VAL	417	86.189	25.247	57.571	1.00 20.00
ATOM	826	N	SER	418	85.433	26.185	53.881	1.00 20.00
ATOM	827	CA	SER	418	84.746	25.369	52.915	1.00 20.00
ATOM	828	C	SER	418	83.262	25.480	53.085	1.00 20.00
ATOM	829	O	SER	418	82.659	24.722	53.844	1.00 20.00
ATOM	830	CB	SER	418	85.129	23.878	52.994	1.00 20.00
ATOM	831	OG	SER	418	86.506	23.711	52.690	1.00 20.00
ATOM	832	N	LEU	419	82.626	26.440	52.377	1.00 40.00
ATOM	833	CA	LEU	419	81.198	26.607	52.499	1.00 40.00
ATOM	834	C	LEU	419	80.599	26.821	51.129	1.00 40.00
ATOM	835	O	LEU	419	81.324	26.980	50.149	1.00 40.00
ATOM	836	CB	LEU	419	80.813	27.822	53.355	1.00 40.00
ATOM	837	CG	LEU	419	81.270	27.699	54.818	1.00 40.00
ATOM	838	CD1	LEU	419	80.866	28.927	55.644	1.00 40.00
ATOM	839	CD2	LEU	419	80.810	26.376	55.444	1.00 40.00
ATOM	840	N	ASN	420	79.246	26.799	51.015	1.00 40.00
ATOM	841	CA	ASN	420	78.582	27.032	49.756	1.00 40.00
ATOM	842	C	ASN	420	77.866	28.337	49.879	1.00 40.00
ATOM	843	O	ASN	420	76.685	28.429	49.637	1.00 40.00
ATOM	844	CB	ASN	420	77.537	25.962	49.404	1.00 40.00
ATOM	845	CG	ASN	420	78.284	24.676	49.001	1.00 40.00
ATOM	846	OD1	ASN	420	77.826	23.580	49.398	1.00 40.00
ATOM	847	ND2	ASN	420	79.471	24.810	48.432	1.00 40.00
ATOM	848	N	ILE	421	78.599	29.408	50.228	1.00 40.00
ATOM	849	CA	ILE	421	77.930	30.654	50.448	1.00 40.00
ATOM	850	C	ILE	421	78.329	31.647	49.411	1.00 40.00
ATOM	851	O	ILE	421	79.478	31.695	48.975	1.00 40.00
ATOM	852	CB	ILE	421	78.234	31.277	51.781	1.00 40.00
ATOM	853	CG1	ILE	421	79.727	31.638	51.901	1.00 40.00
ATOM	854	CG2	ILE	421	77.741	30.314	52.872	1.00 40.00
ATOM	855	CD1	ILE	421	80.670	30.435	51.849	1.00 40.00
ATOM	856	N	THR	422	77.330	32.426	48.948	1.00 20.00
ATOM	857	CA	THR	422	77.505	33.504	48.023	1.00 20.00
ATOM	858	C	THR	422	78.110	34.676	48.736	1.00 20.00
ATOM	859	O	THR	422	78.923	35.399	48.167	1.00 20.00
ATOM	860	CB	THR	422	76.212	33.956	47.406	1.00 20.00
ATOM	861	OG1	THR	422	76.466	34.803	46.361	1.00 20.00
ATOM	862	CG2	THR	422	75.333	34.600	48.491	1.00 20.00
ATOM	863	N	SER	423	77.702	34.922	49.999	1.00 20.00
ATOM	864	CA	SER	423	78.239	36.037	50.731	1.00 20.00
ATOM	865	C	SER	423	78.036	35.761	52.185	1.00 20.00
ATOM	866	O	SER	423	77.447	34.742	52.540	1.00 20.00
ATOM	867	CB	SER	423	77.580	37.380	50.422	1.00 20.00
ATOM	868	OG	SER	423	77.807	37.759	49.078	1.00 20.00
ATOM	869	N	LEU	424	78.604	36.620	53.062	1.00 20.00
ATOM	870	CA	LEU	424	78.421	36.471	54.481	1.00 20.00
ATOM	871	C	LEU	424	77.017	36.647	54.874	1.00 20.00
ATOM	872	O	LEU	424	76.307	36.058	55.689	1.00 20.00
ATOM	873	CB	LEU	424	79.396	37.332	55.300	1.00 20.00
ATOM	874	CG	LEU	424	80.867	36.906	55.136	1.00 20.00
ATOM	875	CD1	LEU	424	81.356	37.119	53.693	1.00 20.00
ATOM	876	CD2	LEU	424	81.768	37.587	56.179	1.00 20.00
ATOM	877	N	GLY	425	76.546	38.060	54.523	1.00 20.00
ATOM	878	CA	GLY	425	75.186	38.410	54.857	1.00 20.00
ATOM	879	C	GLY	425	75.018	38.638	56.342	1.00 20.00
ATOM	880	O	GLY	425	73.901	38.723	56.847	1.00 20.00
ATOM	881	N	LEU	426	76.139	38.702	57.065	1.00 20.00
ATOM	882	CA	LEU	426	76.274	38.987	58.487	1.00 20.00
ATOM	883	C	LEU	426	75.966	40.403	58.841	1.00 20.00

Figure 6 (continued)

ATOM	884	O	LEU	426	76.454	40.879	59.856	1.00 20.00
ATOM	885	CB	LEU	426	77.665	38.670	59.065	1.00 20.00
ATOM	886	CG	LEU	426	77.984	37.186	59.134	1.00 20.00
ATOM	887	CD1	LEU	426	79.351	36.919	59.753	1.00 20.00
ATOM	888	CD2	LEU	426	76.845	36.388	59.817	1.00 20.00
ATOM	889	N	ARG	427	75.213	41.136	58.004	1.00 20.00
ATOM	890	CA	ARG	427	75.050	42.570	58.084	1.00 20.00
ATOM	891	C	ARG	427	74.921	43.120	59.484	1.00 20.00
ATOM	892	O	ARG	427	75.357	44.244	59.721	1.00 20.00
ATOM	893	CB	ARG	427	73.819	43.068	57.306	1.00 20.00
ATOM	894	CG	ARG	427	72.502	42.478	57.815	1.00 20.00
ATOM	895	CD	ARG	427	71.259	43.106	57.181	1.00 20.00
ATOM	896	NE	ARG	427	71.144	44.495	57.707	1.00 20.00
ATOM	897	CZ	ARG	427	70.487	44.719	58.880	1.00 20.00
ATOM	898	NH1	ARG	427	69.939	43.671	59.566	1.00 20.00
ATOM	899	NH2	ARG	427	70.362	45.946	59.367	1.00 20.00
ATOM	900	N	SER	428	74.298	42.408	60.435	1.00 20.00
ATOM	901	CA	SER	428	74.149	42.909	61.783	1.00 20.00
ATOM	902	C	SER	428	75.460	42.961	62.532	1.00 20.00
ATOM	903	O	SER	428	75.575	43.673	63.528	1.00 20.00
ATOM	904	CB	SER	428	73.175	42.073	62.631	1.00 20.00
ATOM	905	OG	SER	428	71.852	42.215	62.138	1.00 20.00
ATOM	906	N	LEU	429	76.467	42.179	62.104	1.00 20.00
ATOM	907	CA	LEU	429	77.715	42.012	62.799	1.00 20.00
ATOM	908	C	LEU	429	78.461	43.309	62.909	1.00 20.00
ATOM	909	O	LEU	429	79.082	43.771	61.954	1.00 20.00
ATOM	910	CB	LEU	429	78.615	40.974	62.104	1.00 20.00
ATOM	911	CG	LEU	429	79.973	40.719	62.780	1.00 20.00
ATOM	912	CD1	LEU	429	79.789	40.131	64.184	1.00 20.00
ATOM	913	CD2	LEU	429	80.876	39.845	61.989	1.00 20.00
ATOM	914	N	LYS	430	78.337	43.962	64.085	1.00 20.00
ATOM	915	CA	LYS	430	78.999	45.194	64.413	1.00 20.00
ATOM	916	C	LYS	430	80.437	45.016	64.804	1.00 20.00
ATOM	917	O	LYS	430	81.300	45.741	64.316	1.00 20.00
ATOM	918	CB	LYS	430	78.307	45.927	65.569	1.00 20.00
ATOM	919	CG	LYS	430	76.908	46.414	65.208	1.00 20.00
ATOM	920	CD	LYS	430	76.894	47.386	64.028	1.00 20.00
ATOM	921	CE	LYS	430	75.571	48.138	63.871	1.00 20.00
ATOM	922	NZ	LYS	430	74.464	47.180	63.585	1.00 20.00
ATOM	923	N	GLU	431	80.758	44.056	65.702	1.00 20.00
ATOM	924	CA	GLU	431	82.132	44.025	66.118	1.00 20.00
ATOM	925	C	GLU	431	82.509	42.685	66.660	1.00 20.00
ATOM	926	O	GLU	431	81.698	41.977	67.258	1.00 20.00
ATOM	927	CB	GLU	431	82.446	45.028	67.241	1.00 20.00
ATOM	928	CG	GLU	431	81.668	44.740	68.528	1.00 20.00
ATOM	929	CD	GLU	431	82.096	45.745	69.589	1.00 20.00
ATOM	930	OE1	GLU	431	82.225	46.950	69.246	1.00 20.00
ATOM	931	OE2	GLU	431	82.303	45.317	70.756	1.00 20.00
ATOM	932	N	ILE	432	83.788	42.315	66.444	1.00 20.00
ATOM	933	CA	ILE	432	84.335	41.119	67.001	1.00 20.00
ATOM	934	C	ILE	432	85.346	41.587	67.993	1.00 20.00
ATOM	935	O	ILE	432	86.495	41.868	67.665	1.00 20.00
ATOM	936	CB	ILE	432	84.984	40.225	65.983	1.00 20.00
ATOM	937	CD1	ILE	432	83.908	39.705	65.013	1.00 20.00
ATOM	938	CG2	ILE	432	85.746	39.111	66.717	1.00 20.00
ATOM	939	CD1	ILE	432	84.454	38.933	63.813	1.00 20.00
ATOM	940	N	SER	433	84.939	41.581	69.269	1.00 20.00
ATOM	941	CA	SER	433	85.652	42.184	70.356	1.00 20.00
ATOM	942	C	SER	433	87.089	41.763	70.341	1.00 20.00
ATOM	943	O	SER	433	87.962	42.579	70.631	1.00 20.00
ATOM	944	CB	SER	433	85.041	41.785	71.709	1.00 20.00
ATOM	945	OG	SER	433	85.756	42.390	72.772	1.00 20.00
ATOM	946	N	ASP	434	87.398	40.491	70.036	1.00 20.00
ATOM	947	CA	ASP	434	88.792	40.137	70.012	1.00 20.00
ATOM	948	C	ASP	434	88.986	39.013	69.053	1.00 20.00
ATOM	949	O	ASP	434	88.073	38.225	68.822	1.00 20.00
ATOM	950	CB	ASP	434	89.345	39.663	71.368	1.00 20.00
ATOM	951	CG	ASP	434	89.544	40.873	72.272	1.00 20.00
ATOM	952	OD1	ASP	434	90.112	41.887	71.787	1.00 20.00
ATOM	953	OD2	ASP	434	89.131	40.797	73.459	1.00 20.00
ATOM	954	N	GLY	435	90.201	38.911	68.475	1.00 20.00
ATOM	955	CA	GLY	435	90.509	37.847	67.569	1.00 20.00
ATOM	956	C	GLY	435	90.299	38.335	66.175	1.00 20.00
ATOM	957	O	GLY	435	89.702	39.386	65.949	1.00 20.00
ATOM	958	N	ASP	436	90.797	37.567	65.201	1.00 20.00
ATOM	959	CA	ASP	436	90.748	37.886	63.811	1.00 20.00
ATOM	960	C	ASP	436	89.743	36.994	63.148	1.00 20.00

Figure 6 (continued)

ATOM	961	O	ASP	436	88.975	36.311	63.820	1.00	20.00
ATOM	962	CB	ASP	436	92.069	37.626	63.148	1.00	20.00
ATOM	963	CG	ASP	436	93.063	38.494	63.935	1.00	20.00
ATOM	964	OD1	ASP	436	92.854	39.736	63.973	1.00	20.00
ATOM	965	OD2	ASP	436	94.027	37.924	64.513	1.00	20.00
ATOM	966	N	VAL	437	89.705	36.998	61.799	1.00	20.00
ATOM	967	CA	VAL	437	88.778	36.153	61.094	1.00	20.00
ATOM	968	C	VAL	437	89.533	35.336	60.083	1.00	20.00
ATOM	969	O	VAL	437	90.631	35.701	59.673	1.00	20.00
ATOM	970	CB	VAL	437	87.706	36.907	60.361	1.00	20.00
ATOM	971	CG1	VAL	437	88.358	37.745	59.251	1.00	20.00
ATOM	972	CG2	VAL	437	86.664	35.904	59.841	1.00	20.00
ATOM	973	N	ILE	438	88.977	34.168	59.687	1.00	20.00
ATOM	974	CA	ILE	438	89.627	33.365	58.695	1.00	20.00
ATOM	975	C	ILE	438	88.610	32.924	57.684	1.00	20.00
ATOM	976	O	ILE	438	87.763	32.072	57.947	1.00	20.00
ATOM	977	CB	ILE	438	90.289	32.125	59.272	1.00	20.00
ATOM	978	CG1	ILE	438	90.967	31.298	58.166	1.00	20.00
ATOM	979	CG2	ILE	438	89.263	31.352	60.116	1.00	20.00
ATOM	980	CD1	ILE	438	92.186	31.974	57.542	1.00	20.00
ATOM	981	N	ILE	439	88.661	33.500	56.470	1.00	20.00
ATOM	982	CA	ILE	439	87.704	33.084	55.485	1.00	20.00
ATOM	983	C	ILE	439	88.464	32.338	54.433	1.00	20.00
ATOM	984	O	ILE	439	89.074	32.941	53.551	1.00	20.00
ATOM	985	CB	ILE	439	87.012	34.237	54.821	1.00	20.00
ATOM	986	CG1	ILE	439	86.286	35.093	55.872	1.00	20.00
ATOM	987	CG2	ILE	439	86.070	33.677	53.742	1.00	20.00
ATOM	988	CD1	ILE	439	85.804	36.437	55.330	1.00	20.00
ATOM	989	N	SER	440	88.421	30.992	54.478	1.00	20.00
ATOM	990	CA	SER	440	89.229	30.270	53.536	1.00	20.00
ATOM	991	C	SER	440	88.437	29.227	52.811	1.00	20.00
ATOM	992	O	SER	440	87.424	28.723	53.291	1.00	20.00
ATOM	993	CB	SER	440	90.421	29.548	54.186	1.00	20.00
ATOM	994	OG	SER	440	89.958	28.629	55.058	1.00	20.00
ATOM	995	N	GLY	441	88.909	28.903	51.590	1.00	20.00
ATOM	996	CA	GLY	441	88.382	27.864	50.778	1.00	20.00
ATOM	997	C	GLY	441	86.915	28.009	50.546	1.00	20.00
ATOM	998	O	GLY	441	86.135	27.138	50.929	1.00	20.00
ATOM	999	N	ASN	442	86.488	29.137	49.944	1.00	20.00
ATOM	1000	CA	ASN	442	85.093	29.274	49.632	1.00	20.00
ATOM	1001	C	ASN	442	85.005	29.741	48.213	1.00	20.00
ATOM	1002	O	ASN	442	84.894	30.937	47.952	1.00	20.00
ATOM	1003	CB	ASN	442	84.401	30.319	50.520	1.00	20.00
ATOM	1004	CG	ASN	442	84.451	29.776	51.941	1.00	20.00
ATOM	1005	OD1	ASN	442	83.812	28.776	52.260	1.00	20.00
ATOM	1006	ND2	ASN	442	85.212	30.441	52.817	1.00	20.00
ATOM	1007	N	LYS	443	84.937	28.795	47.258	1.00	20.00
ATOM	1008	CA	LYS	443	85.043	29.139	45.867	1.00	20.00
ATOM	1009	C	LYS	443	84.022	30.166	45.477	1.00	20.00
ATOM	1010	O	LYS	443	84.353	31.140	44.806	1.00	20.00
ATOM	1011	CB	LYS	443	84.851	27.932	44.933	1.00	20.00
ATOM	1012	CG	LYS	443	84.961	28.283	43.446	1.00	20.00
ATOM	1013	CD	LYS	443	86.362	28.724	43.015	1.00	20.00
ATOM	1014	CE	LYS	443	86.715	30.148	43.450	1.00	20.00
ATOM	1015	NZ	LYS	443	88.081	30.495	42.995	1.00	20.00
ATOM	1016	N	ASN	444	82.761	29.968	45.891	1.00	20.00
ATOM	1017	CA	ASN	444	81.633	30.792	45.550	1.00	20.00
ATOM	1018	C	ASN	444	81.579	32.096	46.295	1.00	20.00
ATOM	1019	O	ASN	444	80.856	32.998	45.877	1.00	20.00
ATOM	1020	CB	ASN	444	80.292	30.080	45.800	1.00	20.00
ATOM	1021	CG	ASN	444	80.205	28.911	44.830	1.00	20.00
ATOM	1022	OD1	ASN	444	80.464	29.057	43.635	1.00	20.00
ATOM	1023	ND2	ASN	444	79.848	27.710	45.358	1.00	20.00
ATOM	1024	N	LEU	445	82.270	32.229	47.442	1.00	20.00
ATOM	1025	CA	LEU	445	82.091	33.401	48.260	1.00	20.00
ATOM	1026	C	LEU	445	82.414	34.664	47.523	1.00	20.00
ATOM	1027	O	LEU	445	83.490	34.830	46.952	1.00	20.00
ATOM	1028	CB	LEU	445	82.912	33.364	49.560	1.00	20.00
ATOM	1029	CG	LEU	445	82.731	34.599	50.488	1.00	20.00
ATOM	1030	CD1	LEU	445	81.271	34.737	50.921	1.00	20.00
ATOM	1031	CD2	LEU	445	83.718	34.585	51.634	1.00	20.00
ATOM	1032	N	CYS	446	81.451	35.606	47.569	1.00	20.00
ATOM	1033	CA	CYS	446	81.490	36.899	46.945	1.00	20.00
ATOM	1034	C	CYS	446	81.246	37.908	48.018	1.00	20.00
ATOM	1035	O	CYS	446	81.101	37.568	49.188	1.00	20.00
ATOM	1036	CB	CYS	446	80.329	37.132	45.973	1.00	20.00
ATOM	1037	SG	CYS	446	80.593	36.880	44.273	1.00	20.00

Figure 6 (continued)

ATOM	1038	N	TYR	447	81.208	39.193	47.621	1.00	20.00
ATOM	1039	CA	TYR	447	80.942	40.263	48.514	1.00	20.00
ATOM	1040	C	TYR	447	81.790	40.152	49.734	1.00	20.00
ATOM	1041	O	TYR	447	81.303	40.330	50.848	1.00	20.00
ATOM	1042	CE	TYR	447	79.468	40.423	48.929	1.00	20.00
ATOM	1043	CG	TYR	447	78.752	40.916	47.703	1.00	20.00
ATOM	1044	CD1	TYR	447	78.867	42.231	47.359	1.00	20.00
ATOM	1045	CD2	TYR	447	77.964	40.074	46.980	1.00	20.00
ATOM	1046	CE1	TYR	447	78.211	42.699	46.274	1.00	20.00
ATOM	1047	CD2	TYR	447	77.306	40.535	45.866	1.00	20.00
ATOM	1048	CZ	TYR	447	77.428	41.847	45.484	1.00	20.00
ATOM	1049	OH	TYR	447	76.749	42.311	44.338	1.00	20.00
ATOM	1050	N	ALA	448	83.035	39.671	49.544	1.00	20.00
ATOM	1051	CA	ALA	448	84.047	39.625	50.560	1.00	20.00
ATOM	1052	C	ALA	448	84.817	40.914	50.607	1.00	20.00
ATOM	1053	O	ALA	448	85.147	41.427	51.676	1.00	20.00
ATOM	1054	CB	ALA	448	85.067	38.499	50.315	1.00	20.00
ATOM	1055	N	ASN	449	85.149	41.438	49.409	1.00	20.00
ATOM	1056	CA	ASN	449	85.956	42.611	49.186	1.00	20.00
ATOM	1057	C	ASN	449	85.186	43.841	49.539	1.00	20.00
ATOM	1058	O	ASN	449	85.757	44.898	49.794	1.00	20.00
ATOM	1059	CB	ASN	449	86.414	42.724	47.726	1.00	20.00
ATOM	1060	CG	ASN	449	87.368	41.562	47.496	1.00	20.00
ATOM	1061	OD1	ASN	449	86.976	40.516	46.981	1.00	20.00
ATOM	1062	ND2	ASN	449	88.653	41.744	47.901	1.00	20.00
ATOM	1063	N	THR	450	83.855	43.710	49.505	1.00	20.00
ATOM	1064	CA	THR	450	82.848	44.704	49.737	1.00	20.00
ATOM	1065	C	THR	450	82.824	45.181	51.165	1.00	20.00
ATOM	1066	O	THR	450	82.274	46.249	51.425	1.00	20.00
ATOM	1067	CB	THR	450	81.487	44.148	49.424	1.00	20.00
ATOM	1068	OG1	THR	450	81.272	42.971	50.188	1.00	20.00
ATOM	1069	CG2	THR	450	81.405	43.804	47.930	1.00	20.00
ATOM	1070	N	ILE	451	83.384	44.407	52.139	1.00	20.00
ATOM	1071	CA	ILE	451	83.195	44.795	53.519	1.00	20.00
ATOM	1072	C	ILE	451	84.451	45.363	54.096	1.00	20.00
ATOM	1073	O	ILE	451	85.564	44.986	53.756	1.00	20.00
ATOM	1074	CB	ILE	451	82.814	43.642	54.403	1.00	20.00
ATOM	1075	CG1	ILE	451	81.477	43.039	53.944	1.00	20.00
ATOM	1076	CG2	ILE	451	82.796	44.140	55.858	1.00	20.00
ATOM	1077	CD1	ILE	451	80.310	44.022	54.008	1.00	20.00
ATOM	1078	N	ASN	452	84.287	46.381	54.997	1.00	20.00
ATOM	1079	CA	ASN	452	85.430	46.946	55.651	1.00	20.00
ATOM	1080	C	ASN	452	85.537	46.312	57.010	1.00	20.00
ATOM	1081	O	ASN	452	84.909	46.715	57.988	1.00	20.00
ATOM	1082	CB	ASN	452	85.415	48.498	55.772	1.00	20.00
ATOM	1083	CG	ASN	452	84.231	49.071	56.598	1.00	20.00
ATOM	1084	OD1	ASN	452	83.264	48.244	56.838	1.00	20.00
ATOM	1085	ND2	ASN	452	84.303	50.246	57.064	1.00	20.00
ATOM	1086	N	TRP	453	86.388	45.283	57.094	1.00	20.00
ATOM	1087	CA	TRP	453	86.577	44.905	58.253	1.00	20.00
ATOM	1088	C	TRP	453	87.207	45.377	59.309	1.00	20.00
ATOM	1089	O	TRP	453	87.187	45.058	60.494	1.00	20.00
ATOM	1090	CB	TRP	453	87.466	43.272	58.049	1.00	20.00
ATOM	1091	CG	TRP	453	86.841	42.273	57.099	1.00	20.00
ATOM	1092	CD1	TRP	453	87.149	42.011	55.795	1.00	20.00
ATOM	1093	CD2	TRP	453	85.737	41.418	57.433	1.00	20.00
ATOM	1094	NE1	TRP	453	86.309	41.042	55.299	1.00	20.00
ATOM	1095	CE2	TRP	453	85.434	40.669	56.296	1.00	20.00
ATOM	1096	CE3	TRP	453	85.027	41.273	58.590	1.00	20.00
ATOM	1097	CZ2	TRP	453	84.414	39.760	56.303	1.00	20.00
ATOM	1098	CZ3	TRP	453	84.004	40.350	58.596	1.00	20.00
ATOM	1099	CH2	TRP	453	83.704	39.608	57.474	1.00	20.00
ATOM	1100	N	LYS	454	87.824	46.487	58.878	1.00	20.00
ATOM	1101	CA	LYS	454	88.483	47.362	59.799	1.00	20.00
ATOM	1102	C	LYS	454	87.483	47.842	60.798	1.00	20.00
ATOM	1103	O	LYS	454	87.787	47.939	61.986	1.00	20.00
ATOM	1104	CB	LYS	454	89.063	48.610	59.116	1.00	20.00
ATOM	1105	CG	LYS	454	90.195	48.302	58.136	1.00	20.00
ATOM	1106	CD	LYS	454	90.542	49.475	57.217	1.00	20.00
ATOM	1107	CE	LYS	454	91.674	49.169	56.236	1.00	20.00
ATOM	1108	NZ	LYS	454	91.903	50.330	55.347	1.00	20.00
ATOM	1109	N	LYS	455	86.261	48.173	60.343	1.00	20.00
ATOM	1110	CA	LYS	455	85.279	48.670	61.258	1.00	20.00
ATOM	1111	C	LYS	455	84.933	47.599	62.247	1.00	20.00
ATOM	1112	O	LYS	455	84.895	47.843	63.452	1.00	20.00
ATOM	1113	CB	LYS	455	83.975	49.093	60.560	1.00	20.00
ATOM	1114	CG	LYS	455	83.005	49.844	61.476	1.00	20.00

Figure 6 (continued)

ATOM	1115	CD	LYS	455	81.875	50.551	60.724	1.00	20.00
ATOM	1116	CE	LYS	455	80.957	51.378	61.626	1.00	20.00
ATOM	1117	NZ	LYS	455	80.231	50.493	62.585	1.00	20.00
ATOM	1118	N	LEU	456	84.693	46.372	61.758	1.00	20.00
ATOM	1119	CA	LEU	456	84.270	45.306	62.627	1.00	20.00
ATOM	1120	C	LEU	456	85.381	44.885	63.545	1.00	20.00
ATOM	1121	O	LEU	456	85.180	44.757	64.752	1.00	20.00
ATOM	1122	CB	LEU	456	83.834	44.040	61.859	1.00	20.00
ATOM	1123	CG	LEU	456	82.586	44.232	61.021	1.00	20.00
ATOM	1124	CD1	LEU	456	82.773	45.256	59.896	1.00	20.00
ATOM	1125	CD2	LEU	456	82.016	42.887	60.510	1.00	20.00
ATOM	1126	N	PHE	457	86.584	44.675	62.995	1.00	20.00
ATOM	1127	CA	PHE	457	87.692	44.185	63.780	1.00	20.00
ATOM	1128	C	PHE	457	88.572	45.337	64.119	1.00	20.00
ATOM	1129	O	PHE	457	89.281	45.659	63.260	1.00	20.00
ATOM	1130	CB	PHE	457	88.622	43.229	63.012	1.00	20.00
ATOM	1131	CG	PHE	457	87.894	41.992	62.626	1.00	20.00
ATOM	1132	CD1	PHE	457	87.867	40.906	63.468	1.00	20.00
ATOM	1133	CD2	PHE	457	87.249	41.919	61.414	1.00	20.00
ATOM	1134	CE1	PHE	457	87.195	39.761	63.103	1.00	20.00
ATOM	1135	CE2	PHE	457	86.580	40.777	61.046	1.00	20.00
ATOM	1136	CZ	PHE	457	86.552	39.695	61.891	1.00	20.00
ATOM	1137	N	GLY	458	88.516	45.793	65.378	1.00	40.00
ATOM	1138	CA	GLY	458	89.413	46.825	65.797	1.00	40.00
ATOM	1139	C	GLY	458	90.750	46.212	66.045	1.00	40.00
ATOM	1140	O	GLY	458	91.788	46.777	65.701	1.00	40.00
ATOM	1141	N	THR	459	90.738	44.999	66.632	1.00	40.00
ATOM	1142	CA	THR	459	91.936	44.364	67.094	1.00	40.00
ATOM	1143	C	THR	459	92.968	44.320	66.017	1.00	40.00
ATOM	1144	O	THR	459	94.062	44.855	66.195	1.00	40.00
ATOM	1145	CB	THR	459	91.699	42.973	67.625	1.00	40.00
ATOM	1146	OG1	THR	459	92.918	42.422	68.100	1.00	40.00
ATOM	1147	CG2	THR	459	91.087	42.065	66.529	1.00	40.00
ATOM	1148	N	SER	460	92.668	43.707	64.857	1.00	40.00
ATOM	1149	CA	SER	460	93.716	43.681	63.885	1.00	40.00
ATOM	1150	C	SER	460	93.211	43.055	62.631	1.00	40.00
ATOM	1151	O	SER	460	93.008	41.845	62.562	1.00	40.00
ATOM	1152	CB	SER	460	94.946	42.869	64.325	1.00	40.00
ATOM	1153	OG	SER	460	95.932	42.890	63.306	1.00	40.00
ATOM	1154	N	GLY	461	92.988	43.894	61.606	1.00	20.00
ATOM	1155	CA	GLY	461	92.549	43.439	60.323	1.00	20.00
ATOM	1156	C	GLY	461	93.676	42.723	59.644	1.00	20.00
ATOM	1157	O	GLY	461	93.459	41.809	58.850	1.00	20.00
ATOM	1158	N	GLN	462	94.924	43.132	59.934	1.00	20.00
ATOM	1159	CA	GLN	462	96.068	42.589	59.250	1.00	20.00
ATOM	1160	C	GLN	462	96.146	41.114	59.504	1.00	20.00
ATOM	1161	O	GLN	462	96.552	40.356	58.625	1.00	20.00
ATOM	1162	CB	GLN	462	97.398	43.204	59.729	1.00	20.00
ATOM	1163	CG	GLN	462	98.619	42.625	59.012	1.00	20.00
ATOM	1164	CD	GLN	462	99.864	43.206	59.562	1.00	20.00
ATOM	1165	OE1	GLN	462	100.784	42.650	60.044	1.00	20.00
ATOM	1166	NE2	GLN	462	99.901	44.663	59.474	1.00	20.00
ATOM	1167	N	LYS	463	95.759	40.681	60.713	1.00	20.00
ATOM	1168	CA	LYS	463	95.867	39.310	61.128	1.00	20.00
ATOM	1169	C	LYS	463	94.938	38.418	60.357	1.00	20.00
ATOM	1170	O	LYS	463	95.195	37.220	60.242	1.00	20.00
ATOM	1171	CB	LYS	463	95.609	39.129	62.625	1.00	20.00
ATOM	1172	CG	LYS	463	96.582	39.909	63.511	1.00	20.00
ATOM	1173	CD	LYS	463	96.052	39.862	63.269	1.00	20.00
ATOM	1174	CE	LYS	463	96.678	40.355	62.120	1.00	20.00
ATOM	1175	NZ	LYS	463	98.788	41.784	62.493	1.00	20.00
ATOM	1176	N	THR	464	93.814	38.949	59.837	1.00	20.00
ATOM	1177	CA	THR	464	92.864	38.124	59.134	1.00	20.00
ATOM	1178	C	THR	464	93.550	37.341	58.060	1.00	20.00
ATOM	1179	O	THR	464	94.479	37.825	57.415	1.00	20.00
ATOM	1180	CB	THR	464	91.764	38.900	58.472	1.00	20.00
ATOM	1181	OG1	THR	464	91.012	39.617	59.441	1.00	20.00
ATOM	1182	CG2	THR	464	90.863	37.917	57.709	1.00	20.00
ATOM	1183	N	LYS	465	93.109	36.080	57.863	1.00	20.00
ATOM	1184	CA	LYS	465	93.702	35.266	56.843	1.00	20.00
ATOM	1185	C	LYS	465	92.636	34.900	55.865	1.00	20.00
ATOM	1186	O	LYS	465	91.615	34.310	56.218	1.00	20.00
ATOM	1187	CB	LYS	465	94.341	33.974	57.380	1.00	20.00
ATOM	1188	CG	LYS	465	95.607	34.234	58.201	1.00	20.00
ATOM	1189	CD	LYS	465	96.091	33.027	59.008	1.00	20.00
ATOM	1190	CE	LYS	465	97.369	33.295	59.806	1.00	20.00
ATOM	1191	NZ	LYS	465	97.091	34.252	60.898	1.00	20.00

Figure 6 (continued)

ATOM	1192	N	ILE	466	92.846	35.262	54.586	1.00	20.00
ATOM	1193	CA	ILE	466	91.846	34.946	53.614	1.00	20.00
ATOM	1194	C	ILE	466	92.517	34.355	52.417	1.00	20.00
ATOM	1195	O	ILE	466	93.466	34.923	51.881	1.00	20.00
ATOM	1196	CB	ILE	466	91.074	36.151	53.170	1.00	20.00
ATOM	1197	CG1	ILE	466	90.332	36.766	54.368	1.00	20.00
ATOM	1198	CG2	ILE	466	90.152	35.737	52.012	1.00	20.00
ATOM	1199	CD1	ILE	466	89.731	38.139	54.078	1.00	20.00
ATOM	1200	N	ILE	467	92.035	33.172	51.984	1.00	20.00
ATOM	1201	CA	ILE	467	92.573	32.536	50.817	1.00	20.00
ATOM	1202	C	ILE	467	91.536	31.584	50.304	1.00	20.00
ATOM	1203	O	ILE	467	90.683	31.122	51.058	1.00	20.00
ATOM	1204	CB	ILE	467	93.788	31.696	51.094	1.00	20.00
ATOM	1205	CG1	ILE	467	93.422	30.547	52.043	1.00	20.00
ATOM	1206	CG2	ILE	467	94.909	32.604	51.623	1.00	20.00
ATOM	1207	CD1	ILE	467	94.498	29.462	52.138	1.00	20.00
ATOM	1208	N	SER	468	91.619	31.255	48.998	1.00	20.00
ATOM	1209	CA	SER	468	90.763	30.284	48.343	1.00	20.00
ATOM	1210	C	SER	468	89.360	30.746	48.165	1.00	20.00
ATOM	1211	O	SER	468	88.467	29.925	47.970	1.00	20.00
ATOM	1212	CB	SER	468	90.779	28.934	49.085	1.00	20.00
ATOM	1213	OG	SER	468	90.070	27.948	48.353	1.00	20.00
ATOM	1214	N	ASN	469	89.097	32.068	48.185	1.00	20.00
ATOM	1215	CA	ASN	469	87.747	32.520	47.969	1.00	20.00
ATOM	1216	C	ASN	469	87.572	32.802	46.507	1.00	20.00
ATOM	1217	O	ASN	469	88.441	32.493	45.693	1.00	20.00
ATOM	1218	CB	ASN	469	87.384	33.794	48.749	1.00	20.00
ATOM	1219	CG	ASN	469	87.287	33.412	50.217	1.00	20.00
ATOM	1220	OD1	ASN	469	86.717	32.378	50.565	1.00	20.00
ATOM	1221	ND2	ASN	469	87.864	34.263	51.106	1.00	20.00
ATOM	1222	N	ARG	470	86.410	33.377	46.130	1.00	20.00
ATOM	1223	CA	ARG	470	86.132	33.660	44.748	1.00	20.00
ATOM	1224	C	ARG	470	86.921	34.869	44.341	1.00	20.00
ATOM	1225	O	ARG	470	87.221	35.734	45.161	1.00	20.00
ATOM	1226	CB	ARG	470	84.637	33.931	44.482	1.00	20.00
ATOM	1227	CG	ARG	470	84.275	34.019	42.999	1.00	20.00
ATOM	1228	CD	ARG	470	82.772	34.139	42.737	1.00	20.00
ATOM	1229	NE	ARG	470	82.588	34.216	41.280	1.00	20.00
ATOM	1230	CZ	ARG	470	81.339	34.380	40.735	1.00	20.00
ATOM	1231	NH1	ARG	470	80.257	34.478	41.562	1.00	20.00
ATOM	1232	NH2	ARG	470	81.173	34.450	39.381	1.00	20.00
ATOM	1233	N	GLY	471	87.287	34.952	43.049	1.00	40.00
ATOM	1234	CA	GLY	471	88.067	36.057	42.562	1.00	40.00
ATOM	1235	C	GLY	471	87.152	37.224	42.377	1.00	40.00
ATOM	1236	O	GLY	471	86.076	37.104	41.795	1.00	40.00
ATOM	1237	N	GLU	472	87.613	38.410	42.811	1.00	40.00
ATOM	1238	CA	GLU	472	86.924	39.608	42.795	1.00	40.00
ATOM	1239	C	GLU	472	86.359	39.843	41.394	1.00	40.00
ATOM	1240	O	GLU	472	85.213	40.227	41.168	1.00	40.00
ATOM	1241	CB	GLU	472	87.656	40.849	43.158	1.00	40.00
ATOM	1242	CG	GLU	472	88.242	40.851	44.569	1.00	40.00
ATOM	1243	CD	GLU	472	89.222	42.008	44.650	1.00	40.00
ATOM	1244	OE1	GLU	472	90.181	42.018	43.832	1.00	40.00
ATOM	1245	OE2	GLU	472	89.027	42.895	45.523	1.00	40.00
ATOM	1246	N	ASN	473	87.251	39.624	40.412	1.00	40.00
ATOM	1247	CA	ASN	473	86.911	39.872	39.041	1.00	40.00
ATOM	1248	C	ASN	473	85.811	38.947	38.630	1.00	40.00
ATOM	1249	O	ASN	473	84.872	39.352	37.944	1.00	40.00
ATOM	1250	CB	ASN	473	88.101	39.653	38.087	1.00	40.00
ATOM	1251	CG	ASN	473	88.545	38.201	38.192	1.00	40.00
ATOM	1252	OD1	ASN	473	88.650	37.650	39.286	1.00	40.00
ATOM	1253	ND2	ASN	473	88.816	37.562	37.022	1.00	40.00
ATOM	1254	N	SER	474	85.903	37.672	39.044	1.00	20.00
ATOM	1255	CA	SER	474	84.930	36.687	38.670	1.00	20.00
ATOM	1256	C	SER	474	83.616	37.035	39.287	1.00	20.00
ATOM	1257	O	SER	474	82.566	36.879	38.667	1.00	20.00
ATOM	1258	CB	SER	474	85.310	35.274	39.145	1.00	20.00
ATOM	1259	OG	SER	474	84.316	34.339	38.752	1.00	20.00
ATOM	1260	N	CYS	475	83.632	37.577	40.538	1.00	20.00
ATOM	1261	CA	CYS	475	82.399	37.791	41.211	1.00	20.00
ATOM	1262	C	CYS	475	81.660	38.870	40.491	1.00	20.00
ATOM	1263	O	CYS	475	80.436	38.823	40.377	1.00	20.00
ATOM	1264	CB	CYS	475	82.545	38.242	42.667	1.00	20.00
ATOM	1265	SG	CYS	475	80.982	38.368	43.562	1.00	20.00
ATOM	1266	N	LYS	476	82.387	39.878	39.979	1.00	60.00
ATOM	1267	CA	LYS	476	81.730	40.949	39.291	1.00	60.00
ATOM	1268	C	LYS	476	80.842	41.650	40.265	1.00	60.00

Figure 6 (continued)

ATOM	1269	O	LYS	476	79.807	42.268	39.902	1.00	60.00
ATOM	1270	CB	LYS	476	80.873	40.477	38.102	1.00	60.00
ATOM	1271	CG	LYS	476	81.696	39.937	36.918	1.00	60.00
ATOM	1272	CD	LYS	476	80.866	39.204	35.876	1.00	60.00
ATOM	1273	CE	LYS	476	81.658	38.812	34.626	1.00	60.00
ATOM	1274	NZ	LYS	476	81.946	40.018	33.814	1.00	60.00
ATOM	1275	N	ALA	477	81.240	41.621	41.647	1.00	60.00
ATOM	1276	CA	ALA	477	80.591	42.330	42.571	1.00	60.00
ATOM	1277	C	ALA	477	81.458	43.425	42.964	1.00	60.00
ATOM	1278	O	ALA	477	82.140	43.988	42.107	1.00	60.00
ATOM	1279	CB	ALA	477	80.270	41.476	43.822	1.00	60.00
ATOM	1280	N	THR	478	81.434	43.761	44.271	1.00	60.00
ATOM	1281	CA	THR	478	82.280	44.706	44.946	1.00	60.00
ATOM	1282	C	THR	478	81.379	45.669	45.645	1.00	60.00
ATOM	1283	O	THR	478	80.150	45.505	45.621	1.00	60.00
ATOM	1284	CB	THR	478	83.241	45.491	44.091	1.00	60.00
ATOM	1285	OG1	THR	478	84.170	46.195	44.906	1.00	60.00
ATOM	1286	CG2	THR	478	82.449	46.475	43.218	1.00	60.00
ATOM	1287	N	GLY	479	81.961	46.668	46.311	1.00	60.00
ATOM	1288	CA	GLY	479	81.135	47.620	46.982	1.00	60.00
ATOM	1289	C	GLY	479	80.339	48.282	45.917	1.00	60.00
ATOM	1290	O	GLY	479	79.229	48.758	46.150	1.00	60.00
ATOM	1291	N	GLN	480	80.915	48.323	44.705	1.00	60.00
ATOM	1292	CA	GLN	480	80.274	48.950	43.583	1.00	60.00
ATOM	1293	C	GLN	480	79.022	48.204	43.269	1.00	60.00
ATOM	1294	O	GLN	480	77.964	48.807	43.111	1.00	60.00
ATOM	1295	CB	GLN	480	81.150	48.968	42.329	1.00	60.00
ATOM	1296	CG	GLN	480	80.508	49.691	41.145	1.00	60.00
ATOM	1297	CD	GLN	480	80.495	51.178	41.465	1.00	60.00
ATOM	1298	OE1	GLN	480	79.907	51.606	42.458	1.00	60.00
ATOM	1299	NE2	GLN	480	81.164	51.981	40.604	1.00	60.00
ATOM	1300	N	VAL	481	79.086	46.867	43.177	1.00	60.00
ATOM	1301	CA	VAL	481	77.874	46.197	42.794	1.00	60.00
ATOM	1302	C	VAL	481	77.040	46.010	44.018	1.00	60.00
ATOM	1303	O	VAL	481	76.809	44.890	44.459	1.00	60.00
ATOM	1304	CB	VAL	481	78.100	44.852	42.165	1.00	60.00
ATOM	1305	CG1	VAL	481	76.738	44.232	41.800	1.00	60.00
ATOM	1306	CG2	VAL	481	79.045	45.029	40.961	1.00	60.00
ATOM	1307	N	CYS	482	76.550	47.117	44.594	1.00	20.00
ATOM	1308	CA	CYS	482	75.700	46.981	45.737	1.00	20.00
ATOM	1309	C	CYS	482	74.501	47.830	45.449	1.00	20.00
ATOM	1310	O	CYS	482	74.309	48.262	44.314	1.00	20.00
ATOM	1311	CB	CYS	482	76.305	47.484	47.059	1.00	20.00
ATOM	1312	SG	CYS	482	75.422	46.745	48.459	1.00	20.00
ATOM	1313	N	HIS	483	73.647	48.093	46.459	1.00	20.00
ATOM	1314	CA	HIS	483	72.490	48.892	46.177	1.00	20.00
ATOM	1315	C	HIS	483	72.962	50.278	45.890	1.00	20.00
ATOM	1316	O	HIS	483	74.064	50.667	46.277	1.00	20.00
ATOM	1317	CB	HIS	483	71.455	48.956	47.314	1.00	20.00
ATOM	1318	CG	HIS	483	70.136	49.489	46.841	1.00	20.00
ATOM	1319	ND1	HIS	483	69.832	50.827	46.731	1.00	20.00
ATOM	1320	CD2	HIS	483	69.027	48.820	46.420	1.00	20.00
ATOM	1321	CE1	HIS	483	68.565	50.902	46.253	1.00	20.00
ATOM	1322	NE2	HIS	483	68.036	49.709	46.048	1.00	20.00
ATOM	1323	N	ALA	484	72.129	51.056	45.177	1.00	20.00
ATOM	1324	CA	ALA	484	72.479	52.397	44.810	1.00	20.00
ATOM	1325	C	ALA	484	72.633	53.183	46.070	1.00	20.00
ATOM	1326	O	ALA	484	73.512	54.036	46.182	1.00	20.00
ATOM	1327	CB	ALA	484	71.397	53.086	43.963	1.00	20.00
ATOM	1328	N	LEU	485	71.761	52.894	47.053	1.00	20.00
ATOM	1329	CA	LEU	485	71.700	53.607	48.296	1.00	20.00
ATOM	1330	C	LEU	485	72.942	53.404	49.104	1.00	20.00
ATOM	1331	O	LEU	485	73.430	54.351	49.719	1.00	20.00
ATOM	1332	CB	LEU	485	70.524	53.126	49.167	1.00	20.00
ATOM	1333	CG	LEU	485	69.159	53.245	48.467	1.00	20.00
ATOM	1334	CD1	LEU	485	68.011	52.771	49.377	1.00	20.00
ATOM	1335	CD2	LEU	485	68.937	54.658	47.908	1.00	20.00
ATOM	1336	N	CYS	486	73.484	52.168	49.133	1.00	20.00
ATOM	1337	CA	CYS	486	74.625	51.904	49.965	1.00	20.00
ATOM	1338	C	CYS	486	75.706	52.850	49.542	1.00	20.00
ATOM	1339	O	CYS	486	75.889	53.172	48.420	1.00	20.00
ATOM	1340	CB	CYS	486	75.216	50.493	49.810	1.00	20.00
ATOM	1341	SG	CYS	486	74.121	49.204	50.457	1.00	20.00
ATOM	1342	N	SER	487	76.426	53.359	50.600	1.00	20.00
ATOM	1343	CA	SER	487	77.514	54.217	50.245	1.00	20.00
ATOM	1344	C	SER	487	78.465	53.328	49.553	1.00	20.00
ATOM	1345	O	SER	487	78.379	52.106	49.660	1.00	20.00

Figure 6 (continued)

ATOM	1346	CB	SER	487	78.281	54.827	51.430	1.00	20.00
ATOM	1347	OG	SER	487	77.478	55.768	52.122	1.00	20.00
ATOM	1348	N	PRO	488	79.382	53.939	48.865	1.00	20.00
ATOM	1349	CA	PRO	488	80.288	53.191	48.173	1.00	20.00
ATOM	1350	C	PRO	488	81.308	52.611	49.194	1.00	20.00
ATOM	1351	O	PRO	488	82.218	51.872	48.822	1.00	20.00
ATOM	1352	CB	PRO	488	81.050	54.175	47.213	1.00	20.00
ATOM	1353	CG	PRO	488	79.936	55.196	46.918	1.00	20.00
ATOM	1354	CD	PRO	488	79.074	55.190	48.190	1.00	20.00
ATOM	1355	N	GLU	489	81.082	52.939	50.480	1.00	20.00
ATOM	1356	CA	GLU	489	81.987	52.429	51.541	1.00	20.00
ATOM	1357	C	GLU	489	81.934	50.937	51.382	1.00	20.00
ATOM	1358	O	GLU	489	83.018	50.363	51.283	1.00	20.00
ATOM	1359	CB	GLU	489	81.309	52.775	52.922	1.00	20.00
ATOM	1360	CG	GLU	489	81.341	54.263	53.271	1.00	20.00
ATOM	1361	CD	GLU	489	82.584	54.519	54.109	1.00	20.00
ATOM	1362	OE1	GLU	489	83.273	53.525	54.462	1.00	20.00
ATOM	1363	OE2	GLU	489	82.857	55.710	54.413	1.00	20.00
ATOM	1364	N	GLY	490	80.767	50.266	51.324	1.00	20.00
ATOM	1365	CA	GLY	490	80.835	48.832	51.130	1.00	20.00
ATOM	1366	C	GLY	490	79.555	48.203	51.585	1.00	20.00
ATOM	1367	O	GLY	490	78.679	48.877	52.122	1.00	20.00
ATOM	1368	N	CYS	491	79.399	46.879	51.350	1.00	20.00
ATOM	1369	CA	CYS	491	78.209	46.235	51.827	1.00	20.00
ATOM	1370	C	CYS	491	78.399	44.758	51.876	1.00	20.00
ATOM	1371	O	CYS	491	79.286	44.211	51.229	1.00	20.00
ATOM	1372	CB	CYS	491	76.949	46.530	50.995	1.00	20.00
ATOM	1373	SG	CYS	491	76.845	45.656	49.412	1.00	20.00
ATOM	1374	N	TRP	492	77.572	44.077	52.696	1.00	20.00
ATOM	1375	CA	TRP	492	77.645	42.652	52.854	1.00	20.00
ATOM	1376	C	TRP	492	77.156	41.956	51.623	1.00	20.00
ATOM	1377	O	TRP	492	77.706	40.931	51.222	1.00	20.00
ATOM	1378	CB	TRP	492	76.839	42.138	54.069	1.00	20.00
ATOM	1379	CG	TRP	492	77.411	42.582	55.386	1.00	20.00
ATOM	1380	CD1	TRP	492	77.066	43.652	56.161	1.00	20.00
ATOM	1381	CD2	TRP	492	78.486	41.917	56.070	1.00	20.00
ATOM	1382	NE1	TRP	492	77.856	43.693	57.285	1.00	20.00
ATOM	1383	CE2	TRP	492	78.736	42.632	57.241	1.00	20.00
ATOM	1384	CZ3	TRP	492	79.206	40.803	55.747	1.00	20.00
ATOM	1385	CZ2	TRP	492	79.715	42.241	58.110	1.00	20.00
ATOM	1386	CH2	TRP	492	80.192	40.412	56.627	1.00	20.00
ATOM	1387	CH2	TRP	492	80.441	41.116	57.786	1.00	20.00
ATOM	1388	N	GLY	493	76.091	42.480	50.992	1.00	20.00
ATOM	1389	CA	GLY	493	75.577	41.039	49.816	1.00	20.00
ATOM	1390	C	GLY	493	74.674	42.826	49.170	1.00	20.00
ATOM	1391	O	GLY	493	74.617	43.940	49.662	1.00	20.00
ATOM	1392	N	PRO	494	74.085	42.479	48.066	1.00	20.00
ATOM	1393	CA	PRO	494	73.181	43.411	47.475	1.00	20.00
ATOM	1394	C	PRO	494	71.957	43.495	48.320	1.00	20.00
ATOM	1395	O	PRO	494	71.244	42.499	48.441	1.00	20.00
ATOM	1396	CB	PRO	494	72.967	42.955	46.028	1.00	20.00
ATOM	1397	CG	PRO	494	73.674	41.587	45.944	1.00	20.00
ATOM	1398	CD	PRO	494	74.719	41.636	47.073	1.00	20.00
ATOM	1399	N	GLU	495	71.693	44.674	48.908	1.00	20.00
ATOM	1400	CA	GLU	495	70.524	44.863	49.712	1.00	20.00
ATOM	1401	C	GLU	495	70.697	46.191	50.372	1.00	20.00
ATOM	1402	O	GLU	495	71.821	46.621	50.624	1.00	20.00
ATOM	1403	CB	GLU	495	70.360	43.811	50.823	1.00	20.00
ATOM	1404	CG	GLU	495	69.053	43.951	51.605	1.00	20.00
ATOM	1405	CD	GLU	495	67.919	43.469	50.712	1.00	20.00
ATOM	1406	OE1	GLU	495	68.141	42.490	49.951	1.00	20.00
ATOM	1407	OE2	GLU	495	66.816	44.076	50.776	1.00	20.00
ATOM	1408	N	PRO	496	69.617	46.867	50.634	1.00	20.00
ATOM	1409	CA	PRO	496	69.728	48.144	51.288	1.00	20.00
ATOM	1410	C	PRO	496	70.094	48.034	52.738	1.00	20.00
ATOM	1411	O	PRO	496	70.527	49.029	53.317	1.00	20.00
ATOM	1412	CB	PRO	496	68.397	48.852	51.047	1.00	20.00
ATOM	1413	CG	PRO	496	67.898	48.245	49.724	1.00	20.00
ATOM	1414	CD	PRO	496	68.500	46.831	49.702	1.00	20.00
ATOM	1415	N	ARG	497	69.850	46.863	53.398	1.00	20.00
ATOM	1416	CA	ARG	497	70.163	46.614	54.740	1.00	20.00
ATOM	1417	C	ARG	497	71.636	46.371	54.907	1.00	20.00
ATOM	1418	O	ARG	497	72.213	46.670	55.950	1.00	20.00
ATOM	1419	CB	ARG	497	69.455	45.366	55.292	1.00	20.00
ATOM	1420	CG	ARG	497	67.933	45.495	55.370	1.00	20.00
ATOM	1421	CD	ARG	497	67.248	44.244	55.923	1.00	20.00
ATOM	1422	NE	ARG	497	65.783	44.307	55.944	1.00	20.00

Figure 6 (continued)

ATOM	1423	CZ	ARG	497	64.915	43.539	55.532	1.00	20.00
ATOM	1424	NH1	ARG	497	65.388	42.340	55.084	1.00	20.00
ATOM	1425	NH2	ARG	497	63.568	43.771	55.562	1.00	20.00
ATOM	1426	N	ASP	498	72.258	45.786	53.871	1.00	20.00
ATOM	1427	CA	ASP	498	73.619	45.318	53.880	1.00	20.00
ATOM	1428	C	ASP	498	74.635	46.415	53.995	1.00	20.00
ATOM	1429	O	ASP	498	75.734	46.167	54.491	1.00	20.00
ATOM	1430	CB	ASP	498	73.972	44.490	52.632	1.00	20.00
ATOM	1431	CG	ASP	498	73.285	43.137	52.760	1.00	20.00
ATOM	1432	OD1	ASP	498	72.794	42.628	53.800	1.00	20.00
ATOM	1433	OD2	ASP	498	73.244	42.594	51.745	1.00	20.00
ATOM	1434	N	CYS	499	74.309	47.632	53.523	1.00	20.00
ATOM	1435	CA	CYS	499	75.217	48.746	53.443	1.00	20.00
ATOM	1436	C	CYS	499	76.076	48.873	54.667	1.00	20.00
ATOM	1437	O	CYS	499	75.673	48.537	55.778	1.00	20.00
ATOM	1438	CB	CYS	499	74.499	50.098	53.319	1.00	20.00
ATOM	1439	SG	CYS	499	73.235	50.139	52.018	1.00	20.00
ATOM	1440	N	VAL	500	77.353	49.258	54.458	1.00	20.00
ATOM	1441	CA	VAL	500	78.214	49.603	55.551	1.00	20.00
ATOM	1442	C	VAL	500	77.873	51.010	55.963	1.00	20.00
ATOM	1443	O	VAL	500	77.909	51.356	57.131	1.00	20.00
ATOM	1444	CB	VAL	500	79.667	49.524	55.206	1.00	20.00
ATOM	1445	CG1	VAL	500	80.029	48.087	54.924	1.00	20.00
ATOM	1446	CG2	VAL	500	79.904	50.443	54.009	1.00	20.00
ATOM	1447	N	SER	501	77.545	51.866	54.552	1.00	20.00
ATOM	1448	CA	SER	501	77.198	53.242	55.189	1.00	20.00
ATOM	1449	C	SER	501	76.137	53.625	54.206	1.00	20.00
ATOM	1450	O	SER	501	75.859	52.874	53.268	1.00	20.00
ATOM	1451	CB	SER	501	78.376	54.213	54.995	1.00	20.00
ATOM	1452	OG	SER	501	77.960	55.545	55.248	1.00	20.00
ATOM	1453	N	CYS	502	75.517	54.815	54.380	1.00	20.00
ATOM	1454	CA	CYS	502	74.431	55.218	53.523	1.00	20.00
ATOM	1455	C	CYS	502	74.844	56.410	52.722	1.00	20.00
ATOM	1456	O	CYS	502	75.623	57.247	53.175	1.00	20.00
ATOM	1457	CB	CYS	502	73.156	55.608	54.284	1.00	20.00
ATOM	1458	SG	CYS	502	72.458	54.244	55.262	1.00	20.00
ATOM	1459	N	ARG	503	74.362	56.473	51.463	1.00	20.00
ATOM	1460	CA	ARG	503	74.650	57.568	50.582	1.00	20.00
ATOM	1461	C	ARG	503	73.932	58.782	51.070	1.00	20.00
ATOM	1462	O	ARG	503	74.479	59.884	51.077	1.00	20.00
ATOM	1463	CB	ARG	503	74.209	57.298	49.134	1.00	20.00
ATOM	1464	CG	ARG	503	74.559	58.432	48.168	1.00	20.00
ATOM	1465	CD	ARG	503	74.376	58.051	46.698	1.00	20.00
ATOM	1466	NE	ARG	503	75.343	56.950	46.414	1.00	20.00
ATOM	1467	CZ	ARG	503	75.391	56.381	45.175	1.00	20.00
ATOM	1468	NH1	ARG	503	74.567	56.830	44.183	1.00	20.00
ATOM	1469	NH2	ARG	503	76.264	55.361	44.929	1.00	20.00
ATOM	1470	N	ASN	504	72.675	58.592	51.510	1.00	20.00
ATOM	1471	CA	ASN	504	71.854	59.676	51.964	1.00	20.00
ATOM	1472	C	ASN	504	71.698	59.517	53.442	1.00	20.00
ATOM	1473	O	ASN	504	72.674	59.580	54.188	1.00	20.00
ATOM	1474	CB	ASN	504	70.443	59.663	51.353	1.00	20.00
ATOM	1475	CG	ASN	504	70.559	60.054	49.887	1.00	20.00
ATOM	1476	OD1	ASN	504	70.337	61.208	49.524	1.00	20.00
ATOM	1477	ND2	ASN	504	70.931	59.074	49.021	1.00	20.00
ATOM	1478	N	VAL	505	70.445	59.326	53.902	1.00	20.00
ATOM	1479	CA	VAL	505	70.183	59.225	55.308	1.00	20.00
ATOM	1480	C	VAL	505	69.850	57.813	55.663	1.00	20.00
ATOM	1481	O	VAL	505	69.209	57.094	54.899	1.00	20.00
ATOM	1482	CB	VAL	505	69.023	60.068	55.753	1.00	20.00
ATOM	1483	CG1	VAL	505	69.370	61.547	55.508	1.00	20.00
ATOM	1484	CG2	VAL	505	67.760	59.592	55.015	1.00	20.00
ATOM	1485	N	SER	506	70.288	57.376	56.861	1.00	20.00
ATOM	1486	CA	SER	506	70.013	56.032	57.274	1.00	20.00
ATOM	1487	C	SER	506	68.874	56.071	58.232	1.00	20.00
ATOM	1488	O	SER	506	68.829	56.923	59.116	1.00	20.00
ATOM	1489	CB	SER	506	71.196	55.346	57.979	1.00	20.00
ATOM	1490	OG	SER	506	71.513	56.029	59.184	1.00	20.00
ATOM	1491	N	ARG	507	67.889	55.167	58.054	1.00	20.00
ATOM	1492	CA	ARG	507	66.805	55.162	58.986	1.00	20.00
ATOM	1493	C	ARG	507	66.316	53.760	59.162	1.00	20.00
ATOM	1494	O	ARG	507	66.135	53.024	58.195	1.00	20.00
ATOM	1495	CB	ARG	507	65.582	55.976	58.540	1.00	20.00
ATOM	1496	CG	ARG	507	64.569	56.137	59.674	1.00	20.00
ATOM	1497	CD	ARG	507	63.128	56.325	59.207	1.00	20.00
ATOM	1498	NE	ARG	507	62.640	54.978	58.799	1.00	20.00
ATOM	1499	CZ	ARG	507	62.196	54.103	59.749	1.00	20.00

Figure 6 (continued)

ATOM	1500	NH1	ARG	507	62.193	54.466	61.063	1.00	20.00
ATOM	1501	NH2	ARG	507	61.767	52.860	59.384	1.00	20.00
ATOM	1502	N	GLY	508	66.092	53.353	60.427	1.00	20.00
ATOM	1503	CA	GLY	508	65.512	52.070	60.708	1.00	20.00
ATOM	1504	C	GLY	508	66.299	50.986	60.045	1.00	20.00
ATOM	1505	O	GLY	508	65.752	50.122	59.379	1.00	20.00
ATOM	1506	N	ARG	509	67.634	51.005	60.199	1.00	20.00
ATOM	1507	CA	ARG	509	68.449	49.952	59.663	1.00	20.00
ATOM	1508	C	ARG	509	68.364	49.934	58.167	1.00	20.00
ATOM	1509	O	ARG	509	68.854	48.989	57.537	1.00	20.00
ATOM	1510	CB	ARG	509	68.034	48.563	60.175	1.00	20.00
ATOM	1511	CG	ARG	509	68.317	48.359	61.665	1.00	20.00
ATOM	1512	CD	ARG	509	67.553	49.333	62.566	1.00	20.00
ATOM	1513	NE	ARG	509	67.924	49.017	63.973	1.00	20.00
ATOM	1514	CZ	ARG	509	68.352	50.012	64.803	1.00	20.00
ATOM	1515	NH1	ARG	509	68.460	51.291	64.334	1.00	20.00
ATOM	1516	NH2	ARG	509	68.685	49.728	66.097	1.00	20.00
ATOM	1517	N	GLU	510	67.772	50.970	57.542	1.00	20.00
ATOM	1518	CA	GLU	510	67.718	50.937	56.106	1.00	20.00
ATOM	1519	C	GLU	510	68.333	52.195	55.588	1.00	20.00
ATOM	1520	O	GLU	510	68.194	53.259	56.189	1.00	20.00
ATOM	1521	CB	GLU	510	66.288	50.867	55.645	1.00	20.00
ATOM	1522	CG	GLU	510	65.582	49.546	55.849	1.00	20.00
ATOM	1523	CD	GLU	510	64.187	49.607	55.244	1.00	20.00
ATOM	1524	OE1	GLU	510	63.465	50.600	55.520	1.00	20.00
ATOM	1525	OE2	GLU	510	63.828	48.660	54.492	1.00	20.00
ATOM	1526	N	CYS	511	69.047	52.103	54.447	1.00	20.00
ATOM	1527	CA	CYS	511	69.634	53.269	53.898	1.00	20.00
ATOM	1528	C	CYS	511	68.588	53.937	53.058	1.00	20.00
ATOM	1529	O	CYS	511	68.168	53.366	52.050	1.00	20.00
ATOM	1530	CB	CYS	511	70.861	53.056	53.004	1.00	20.00
ATOM	1531	SG	CYS	511	72.367	52.696	53.951	1.00	20.00
ATOM	1532	N	VAL	512	68.147	55.145	53.455	1.00	20.00
ATOM	1533	CA	VAL	512	67.083	55.770	52.731	1.00	20.00
ATOM	1534	C	VAL	512	67.616	56.996	52.045	1.00	20.00
ATOM	1535	O	VAL	512	68.571	57.622	52.500	1.00	20.00
ATOM	1536	CB	VAL	512	65.925	56.163	53.592	1.00	20.00
ATOM	1537	CG1	VAL	512	64.874	56.802	52.679	1.00	20.00
ATOM	1538	CG2	VAL	512	65.431	54.930	54.370	1.00	20.00
ATOM	1539	N	ASP	513	67.031	57.324	50.876	1.00	20.00
ATOM	1540	CA	ASP	513	67.399	58.471	50.092	1.00	20.00
ATOM	1541	C	ASP	513	66.971	59.731	50.782	1.00	20.00
ATOM	1542	O	ASP	513	67.655	60.757	50.705	1.00	20.00
ATOM	1543	CB	ASP	513	66.741	58.477	48.701	1.00	20.00
ATOM	1544	CG	ASP	513	67.445	57.430	47.852	1.00	20.00
ATOM	1545	OD1	ASP	513	68.703	57.390	47.899	1.00	20.00
ATOM	1546	OD2	ASP	513	66.739	56.654	47.153	1.00	20.00
ATOM	1547	N	LYS	514	65.792	59.711	51.433	1.00	20.00
ATOM	1548	CA	LYS	514	65.328	60.890	52.111	1.00	20.00
ATOM	1549	C	LYS	514	64.841	60.445	53.303	1.00	20.00
ATOM	1550	O	LYS	514	64.072	59.314	53.363	1.00	20.00
ATOM	1551	CB	LYS	514	64.418	61.783	51.250	1.00	20.00
ATOM	1552	CG	LYS	514	65.171	62.493	50.121	1.00	20.00
ATOM	1553	CD	LYS	514	64.262	63.132	49.070	1.00	20.00
ATOM	1554	CE	LYS	514	65.032	63.843	47.956	1.00	20.00
ATOM	1555	NZ	LYS	514	64.091	64.362	46.939	1.00	20.00
ATOM	1556	N	CYS	515	64.364	61.331	54.298	1.00	20.00
ATOM	1557	CA	CYS	515	63.702	60.901	55.494	1.00	20.00
ATOM	1558	C	CYS	515	62.260	60.630	55.213	1.00	20.00
ATOM	1559	O	CYS	515	61.617	61.322	54.424	1.00	20.00
ATOM	1560	CB	CYS	515	63.779	61.925	56.639	1.00	20.00
ATOM	1561	SG	CYS	515	65.495	62.245	57.135	1.00	20.00
ATOM	1562	N	LYS	516	61.715	59.587	55.874	1.00	20.00
ATOM	1563	CA	LYS	516	60.338	59.248	55.681	1.00	20.00
ATOM	1564	C	LYS	516	59.508	60.268	56.388	1.00	20.00
ATOM	1565	O	LYS	516	60.028	61.176	57.034	1.00	20.00
ATOM	1566	CB	LYS	516	59.937	57.853	56.196	1.00	20.00
ATOM	1567	CG	LYS	516	60.407	56.721	55.201	1.00	20.00
ATOM	1568	CD	LYS	516	60.131	55.319	55.828	1.00	20.00
ATOM	1569	CE	LYS	516	60.375	54.214	54.799	1.00	20.00
ATOM	1570	NZ	LYS	516	59.995	52.899	55.363	1.00	20.00
ATOM	1571	N	LEU	517	58.173	60.138	56.266	1.00	20.00
ATOM	1572	CA	LEU	517	57.262	61.090	56.830	1.00	20.00
ATOM	1573	C	LEU	517	57.420	61.100	58.318	1.00	20.00
ATOM	1574	O	LEU	517	57.760	60.087	58.929	1.00	20.00
ATOM	1575	CB	LEU	517	55.786	60.760	56.550	1.00	20.00
ATOM	1576	CG	LEU	517	55.421	60.732	55.055	1.00	20.00

Figure 6 (continued)

ATOM	1577	CD1	LEU	517	53.936	60.393	54.852	1.00 20.00
ATOM	1578	CD2	LEU	517	55.842	62.028	54.350	1.00 20.00
ATOM	1579	N	LEU	518	57.184	62.278	58.926	1.00 20.00
ATOM	1580	CA	LEU	518	57.206	62.441	60.351	1.00 20.00
ATOM	1581	C	LEU	518	58.616	62.527	60.845	1.00 20.00
ATOM	1582	O	LEU	518	58.919	63.348	61.710	1.00 20.00
ATOM	1583	CB	LEU	518	56.481	61.310	61.099	1.00 20.00
ATOM	1584	CG	LEU	518	54.964	61.303	60.837	1.00 20.00
ATOM	1585	CD1	LEU	518	54.269	60.161	61.598	1.00 20.00
ATOM	1586	CD2	LEU	518	54.346	62.679	61.130	1.00 20.00
ATOM	1587	N	GLU	519	59.531	61.699	60.306	1.00 20.00
ATOM	1588	CA	GLU	519	60.877	61.766	60.797	1.00 20.00
ATOM	1589	C	GLU	519	61.592	62.939	60.067	1.00 20.00
ATOM	1590	O	GLU	519	61.258	63.149	58.904	1.00 20.00
ATOM	1591	CB	GLU	519	61.672	60.458	60.647	1.00 20.00
ATOM	1592	CG	GLU	519	61.236	59.365	61.674	1.00 20.00
ATOM	1593	CD	GLU	519	59.893	58.814	61.315	1.00 20.00
ATOM	1594	OE1	GLU	519	59.860	58.108	60.134	1.00 20.00
ATOM	1595	OE2	GLU	519	58.880	59.092	61.872	1.00 20.00
ATOM	1596	N	GLY	520	62.600	63.450	60.700	1.00 20.00
ATOM	1597	CA	GLY	520	63.343	64.505	60.084	1.00 20.00
ATOM	1598	C	GLY	520	64.786	64.197	60.269	1.00 20.00
ATOM	1599	O	GLY	520	65.170	63.520	61.219	1.00 20.00
ATOM	1600	N	GLU	521	65.634	64.696	59.351	1.00 20.00
ATOM	1601	CA	GLU	521	67.033	64.438	59.482	1.00 20.00
ATOM	1602	C	GLU	521	67.477	65.134	60.722	1.00 20.00
ATOM	1603	O	GLU	521	67.161	66.299	60.953	1.00 20.00
ATOM	1604	CB	GLU	521	67.854	64.944	58.281	1.00 20.00
ATOM	1605	CG	GLU	521	67.662	66.433	57.990	1.00 20.00
ATOM	1606	CD	GLU	521	68.339	66.736	56.660	1.00 20.00
ATOM	1607	OE1	GLU	521	68.965	65.804	56.089	1.00 20.00
ATOM	1608	OE2	GLU	521	68.232	67.902	56.194	1.00 20.00
ATOM	1609	N	PRO	522	68.191	64.445	61.571	1.00 40.00
ATOM	1610	CA	PRO	522	68.590	65.051	62.816	1.00 40.00
ATOM	1611	C	PRO	522	69.641	66.105	62.691	1.00 40.00
ATOM	1612	O	PRO	522	70.631	65.986	61.995	1.00 40.00
ATOM	1613	CB	PRO	522	68.963	63.902	63.758	1.00 40.00
ATOM	1614	CG	PRO	522	68.931	62.640	62.873	1.00 40.00
ATOM	1615	CD	PRO	522	67.980	63.018	61.729	1.00 40.00
ATOM	1616	N	ARG	523	69.439	67.259	63.361	1.00 60.00
ATOM	1617	CA	ARG	523	70.404	68.317	63.323	1.00 60.00
ATOM	1618	C	ARG	523	71.616	67.918	64.106	1.00 60.00
ATOM	1619	O	ARG	523	72.742	68.050	63.637	1.00 60.00
ATOM	1620	CB	ARG	523	69.898	69.639	63.931	1.00 60.00
ATOM	1621	CG	ARG	523	70.919	70.776	63.818	1.00 60.00
ATOM	1622	CD	ARG	523	70.536	72.058	64.564	1.00 60.00
ATOM	1623	NE	ARG	523	71.636	73.041	64.343	1.00 60.00
ATOM	1624	CZ	ARG	523	71.887	74.014	65.267	1.00 60.00
ATOM	1625	NH1	ARG	523	71.129	74.090	66.400	1.00 60.00
ATOM	1626	NH2	ARG	523	72.906	74.921	65.068	1.00 60.00
ATOM	1627	N	GLU	524	71.410	67.395	65.334	1.00 60.00
ATOM	1628	CA	GLU	524	72.537	67.073	66.160	1.00 60.00
ATOM	1629	C	GLU	524	73.343	66.039	65.461	1.00 60.00
ATOM	1630	O	GLU	524	74.560	66.165	65.332	1.00 60.00
ATOM	1631	CB	GLU	524	72.162	66.483	67.533	1.00 60.00
ATOM	1632	CG	GLU	524	71.570	67.491	68.523	1.00 60.00
ATOM	1633	CD	GLU	524	70.085	67.643	68.235	1.00 60.00
ATOM	1634	OE1	GLU	524	69.607	67.051	67.231	1.00 60.00
ATOM	1635	OE2	GLU	524	69.406	68.354	69.023	1.00 60.00
ATOM	1636	N	PHE	525	72.674	64.984	64.971	1.00 60.00
ATOM	1637	CA	PHE	525	73.418	63.963	64.305	1.00 60.00
ATOM	1638	C	PHE	525	73.617	64.492	62.925	1.00 60.00
ATOM	1639	O	PHE	525	73.082	65.545	62.585	1.00 60.00
ATOM	1640	CB	PHE	525	72.657	62.627	64.219	1.00 60.00
ATOM	1641	CG	PHE	525	73.668	61.556	64.006	1.00 60.00
ATOM	1642	CD1	PHE	525	74.325	61.016	65.090	1.00 60.00
ATOM	1643	CD2	PHE	525	73.963	61.087	62.748	1.00 60.00
ATOM	1644	CE1	PHE	525	75.264	60.028	64.924	1.00 60.00
ATOM	1645	CE2	PHE	525	74.903	60.099	62.579	1.00 60.00
ATOM	1646	CZ	PHE	525	75.555	59.567	63.664	1.00 60.00
ATOM	1647	N	VAL	526	74.415	63.797	62.095	1.00 60.00
ATOM	1648	CA	VAL	526	74.595	64.304	60.771	1.00 60.00
ATOM	1649	C	VAL	526	73.243	64.306	60.144	1.00 60.00
ATOM	1650	O	VAL	526	72.482	63.349	60.278	1.00 60.00
ATOM	1651	CB	VAL	526	75.510	63.469	59.921	1.00 60.00
ATOM	1652	CG1	VAL	526	75.562	64.081	58.511	1.00 60.00
ATOM	1653	CG2	VAL	526	76.883	63.396	60.612	1.00 60.00

Figure 6 (continued)

ATOM	1654	N	GLU	527	72.897	65.409	59.458	1.00	60.00
ATOM	1655	CA	GLU	527	71.597	65.488	58.869	1.00	60.00
ATOM	1656	C	GLU	527	71.514	64.370	57.891	1.00	60.00
ATOM	1657	O	GLU	527	70.546	63.613	57.861	1.00	60.00
ATOM	1658	CB	GLU	527	71.392	66.788	58.072	1.00	60.00
ATOM	1659	CG	GLU	527	71.414	68.055	56.928	1.00	60.00
ATOM	1660	CD	GLU	527	71.252	69.250	57.999	1.00	60.00
ATOM	1661	OE1	GLU	527	71.085	69.028	56.770	1.00	60.00
ATOM	1662	OE2	GLU	527	71.293	70.403	58.506	1.00	60.00
ATOM	1663	N	ASN	528	72.567	64.240	57.068	1.00	60.00
ATOM	1664	CA	ASN	528	72.618	63.234	56.060	1.00	60.00
ATOM	1665	C	ASN	528	72.710	61.890	56.701	1.00	60.00
ATOM	1666	O	ASN	528	72.087	60.941	56.241	1.00	60.00
ATOM	1667	CB	ASN	528	73.838	63.374	55.135	1.00	60.00
ATOM	1668	CG	ASN	528	73.641	64.626	54.287	1.00	60.00
ATOM	1669	OD1	ASN	528	74.432	65.565	54.344	1.00	60.00
ATOM	1670	ND2	ASN	528	72.552	64.636	53.473	1.00	60.00
ATOM	1671	N	SER	529	73.478	61.760	57.793	1.00	60.00
ATOM	1672	CA	SER	529	73.716	60.445	58.313	1.00	60.00
ATOM	1673	C	SER	529	72.448	59.746	58.702	1.00	60.00
ATOM	1674	O	SER	529	72.248	58.593	58.323	1.00	60.00
ATOM	1675	CB	SER	529	74.643	60.435	59.538	1.00	60.00
ATOM	1676	OG	SER	529	74.829	59.100	59.984	1.00	60.00
ATOM	1677	N	GLU	530	71.541	60.397	59.456	1.00	40.00
ATOM	1678	CA	GLU	530	70.397	59.636	59.881	1.00	40.00
ATOM	1679	C	GLU	530	69.179	60.502	59.862	1.00	40.00
ATOM	1680	O	GLU	530	69.253	61.698	59.585	1.00	40.00
ATOM	1681	CB	GLU	530	70.544	59.105	61.320	1.00	40.00
ATOM	1682	CG	GLU	530	69.478	58.099	61.765	1.00	40.00
ATOM	1683	CD	GLU	530	69.711	57.756	63.212	1.00	40.00
ATOM	1684	OE1	GLU	530	70.606	58.395	63.829	1.00	40.00
ATOM	1685	OE2	GLU	530	68.993	56.865	63.737	1.00	40.00
ATOM	1686	N	CYS	531	68.010	59.880	60.133	1.00	20.00
ATOM	1687	CA	CYS	531	66.759	60.567	60.248	1.00	20.00
ATOM	1688	C	CYS	531	66.246	60.216	61.610	1.00	20.00
ATOM	1689	O	CYS	531	66.410	59.086	62.065	1.00	20.00
ATOM	1690	CB	CYS	531	65.703	60.088	59.241	1.00	20.00
ATOM	1691	SG	CYS	531	66.199	60.382	57.521	1.00	20.00
ATOM	1692	N	ILE	532	65.626	61.184	62.311	1.00	20.00
ATOM	1693	CA	ILE	532	65.117	60.898	63.621	1.00	20.00
ATOM	1694	C	ILE	532	63.678	61.295	63.671	1.00	20.00
ATOM	1695	O	ILE	532	63.192	62.029	62.815	1.00	20.00
ATOM	1696	CB	ILE	532	65.823	61.617	64.733	1.00	20.00
ATOM	1697	CG1	ILE	532	65.724	63.139	64.540	1.00	20.00
ATOM	1698	CG2	ILE	532	67.251	61.058	64.841	1.00	20.00
ATOM	1699	CD1	ILE	532	66.167	63.939	65.763	1.00	20.00
ATOM	1700	N	GLN	533	62.951	60.788	64.086	1.00	20.00
ATOM	1701	CA	GLN	533	61.553	61.067	64.413	1.00	20.00
ATOM	1702	C	GLN	533	61.371	62.413	65.417	1.00	20.00
ATOM	1703	O	GLN	533	62.119	62.823	66.302	1.00	20.00
ATOM	1704	CB	GLN	533	60.804	60.067	65.701	1.00	20.00
ATOM	1705	CG	GLN	533	60.794	58.634	65.136	1.00	20.00
ATOM	1706	CD	GLN	533	60.037	57.743	66.106	1.00	20.00
ATOM	1707	OE1	GLN	533	60.333	57.691	67.296	1.00	20.00
ATOM	1708	NE2	GLN	533	59.003	57.022	65.581	1.00	20.00
ATOM	1709	N	CYS	534	60.367	63.148	64.910	1.00	20.00
ATOM	1710	CA	CYS	534	60.022	64.403	65.495	1.00	20.00
ATOM	1711	C	CYS	534	58.574	64.280	65.865	1.00	20.00
ATOM	1712	O	CYS	534	57.948	63.256	65.598	1.00	20.00
ATOM	1713	CB	CYS	534	60.157	65.644	64.582	1.00	20.00
ATOM	1714	SG	CYS	534	61.866	66.147	64.183	1.00	20.00
ATOM	1715	N	HIS	535	58.003	65.315	66.513	1.00	20.00
ATOM	1716	CA	HIS	535	56.617	65.244	66.889	1.00	20.00
ATOM	1717	C	HIS	535	55.831	65.268	65.620	1.00	20.00
ATOM	1718	O	HIS	535	56.310	65.745	64.593	1.00	20.00
ATOM	1719	CB	HIS	535	56.161	66.422	67.770	1.00	20.00
ATOM	1720	CG	HIS	535	54.770	66.262	68.309	1.00	20.00
ATOM	1721	ND1	HIS	535	53.636	66.718	67.675	1.00	20.00
ATOM	1722	CD2	HIS	535	54.340	65.670	69.457	1.00	20.00
ATOM	1723	CE1	HIS	535	52.584	66.385	68.464	1.00	20.00
ATOM	1724	NE2	HIS	535	52.961	65.742	69.556	1.00	20.00
ATOM	1725	N	PRO	536	54.644	64.732	65.647	1.00	20.00
ATOM	1726	CA	PRO	536	53.823	64.689	64.473	1.00	20.00
ATOM	1727	C	PRO	536	53.461	66.068	64.022	1.00	20.00
ATOM	1728	O	PRO	536	53.280	66.271	62.822	1.00	20.00
ATOM	1729	CB	PRO	536	52.638	63.781	64.819	1.00	20.00
ATOM	1730	CG	PRO	536	52.756	63.534	66.339	1.00	20.00

Figure 6 (continued)

ATOM	1731	CD	PRO	536	54.250	63.742	66.631	1.00	20.00
ATOM	1732	N	GLU	537	53.317	67.015	64.965	1.00	20.00
ATOM	1733	CA	GLU	537	52.970	66.366	64.641	1.00	20.00
ATOM	1734	C	GLU	537	54.125	69.112	64.053	1.00	20.00
ATOM	1735	O	GLU	537	53.932	69.949	63.171	1.00	20.00
ATOM	1736	CB	GLU	537	52.434	69.166	65.841	1.00	20.00
ATOM	1737	CG	GLU	537	51.026	68.734	66.257	1.00	20.00
ATOM	1738	CD	GLU	537	50.080	69.061	65.105	1.00	20.00
ATOM	1739	OE1	GLU	537	50.515	69.775	64.162	1.00	20.00
ATOM	1740	OE2	GLU	537	48.909	68.599	65.157	1.00	20.00
ATOM	1741	N	CYS	538	55.359	68.847	64.529	1.00	20.00
ATOM	1742	CA	CYS	538	56.479	69.589	64.027	1.00	20.00
ATOM	1743	C	CYS	538	56.535	69.399	62.554	1.00	20.00
ATOM	1744	O	CYS	538	56.200	68.330	62.059	1.00	20.00
ATOM	1745	CB	CYS	538	57.849	69.144	64.565	1.00	20.00
ATOM	1746	SG	CYS	538	58.114	69.567	66.305	1.00	20.00
ATOM	1747	N	LEU	539	56.913	70.467	61.832	1.00	40.00
ATOM	1748	CA	LEU	539	57.049	70.324	60.421	1.00	40.00
ATOM	1749	C	LEU	539	58.467	70.668	60.113	1.00	40.00
ATOM	1750	O	LEU	539	58.920	71.783	60.360	1.00	40.00
ATOM	1751	CB	LEU	539	56.156	71.279	59.613	1.00	40.00
ATOM	1752	CG	LEU	539	56.308	71.113	58.090	1.00	40.00
ATOM	1753	CD1	LEU	539	55.841	69.723	57.627	1.00	40.00
ATOM	1754	CD2	LEU	539	55.618	72.257	57.330	1.00	40.00
ATOM	1755	N	PRO	540	59.166	69.715	59.576	1.00	60.00
ATOM	1756	CA	PRO	540	60.536	69.937	59.213	1.00	60.00
ATOM	1757	C	PRO	540	60.630	70.650	57.905	1.00	60.00
ATOM	1758	O	PRO	540	59.692	70.573	57.113	1.00	60.00
ATOM	1759	CB	PRO	540	61.269	68.661	59.211	1.00	60.00
ATOM	1760	CG	PRO	540	60.042	67.557	59.204	1.00	60.00
ATOM	1761	CD	PRO	540	58.906	68.323	59.898	1.00	60.00
ATOM	1762	N	GLN	541	61.752	71.357	57.667	1.00	60.00
ATOM	1763	CA	GLN	541	61.955	72.030	56.420	1.00	60.00
ATOM	1764	C	GLN	541	63.198	71.447	55.840	1.00	60.00
ATOM	1765	O	GLN	541	64.142	71.139	56.564	1.00	60.00
ATOM	1766	CB	GLN	541	62.189	73.543	56.560	1.00	60.00
ATOM	1767	CG	GLN	541	60.949	74.310	57.026	1.00	60.00
ATOM	1768	CD	GLN	541	59.944	74.291	55.883	1.00	60.00
ATOM	1769	OE1	GLN	541	59.626	73.234	55.340	1.00	60.00
ATOM	1770	NE2	GLN	541	59.436	75.492	55.500	1.00	60.00
ATOM	1771	N	ALA	542	63.223	71.245	54.511	1.00	60.00
ATOM	1772	CA	ALA	542	64.400	70.665	53.941	1.00	60.00
ATOM	1773	C	ALA	542	65.538	71.612	54.146	1.00	60.00
ATOM	1774	O	ALA	542	66.570	71.247	54.706	1.00	60.00
ATOM	1775	CB	ALA	542	64.271	70.421	52.428	1.00	60.00
ATOM	1776	N	MET	543	65.368	72.872	53.701	1.00	60.00
ATOM	1777	CA	MET	543	66.419	73.835	53.841	1.00	60.00
ATOM	1778	C	MET	543	66.577	74.177	55.283	1.00	60.00
ATOM	1779	O	MET	543	67.692	74.256	55.799	1.00	60.00
ATOM	1780	CB	MET	543	66.151	75.148	53.086	1.00	60.00
ATOM	1781	CG	MET	543	67.326	76.128	53.160	1.00	60.00
ATOM	1782	SD	MET	543	67.069	77.701	52.287	1.00	60.00
ATOM	1783	CE	MET	543	68.699	78.360	52.710	1.00	60.00
ATOM	1784	N	ASN	544	65.443	74.378	55.976	1.00	60.00
ATOM	1785	CA	ASN	544	65.489	74.780	57.349	1.00	60.00
ATOM	1786	C	ASN	544	65.876	73.603	58.174	1.00	60.00
ATOM	1787	O	ASN	544	65.982	72.482	57.681	1.00	60.00
ATOM	1788	CB	ASN	544	64.147	75.310	57.893	1.00	60.00
ATOM	1789	CG	ASN	544	63.857	76.629	57.180	1.00	60.00
ATOM	1790	OD1	ASN	544	63.812	76.694	55.952	1.00	60.00
ATOM	1791	ND2	ASN	544	63.657	77.711	57.977	1.00	60.00
ATOM	1792	N	ILE	545	66.130	73.853	59.470	1.00	60.00
ATOM	1793	CA	ILE	545	66.510	72.802	60.358	1.00	60.00
ATOM	1794	C	ILE	545	65.274	72.045	60.699	1.00	60.00
ATOM	1795	O	ILE	545	64.176	72.384	60.262	1.00	60.00
ATOM	1796	CB	ILE	545	67.099	73.290	61.649	1.00	60.00
ATOM	1797	CG1	ILE	545	66.061	74.113	62.430	1.00	60.00
ATOM	1798	CG2	ILE	545	68.389	74.066	61.325	1.00	60.00
ATOM	1799	CD1	ILE	545	66.466	74.394	63.876	1.00	60.00
ATOM	1800	N	THR	546	65.441	70.974	61.493	1.00	40.00
ATOM	1801	CA	THR	546	64.335	70.165	61.904	1.00	40.00
ATOM	1802	C	THR	546	64.240	70.322	63.381	1.00	40.00
ATOM	1803	O	THR	546	64.991	71.105	63.966	1.00	40.00
ATOM	1804	CB	THR	546	64.522	68.703	61.620	1.00	40.00
ATOM	1805	OG1	THR	546	63.322	67.992	61.887	1.00	40.00
ATOM	1806	CG2	THR	546	65.667	68.171	62.499	1.00	40.00
ATOM	1807	N	CYS	547	63.289	69.606	64.012	1.00	20.00

Figure 6 (continued)

ATOM	1808	CA	CYS	547	63.128	69.673	65.427	1.00	20.00
ATOM	1809	C	CYS	547	64.449	69.456	66.074	1.00	20.00
ATOM	1810	O	CYS	547	65.206	68.567	65.694	1.00	20.00
ATOM	1811	CB	CYS	547	62.115	68.643	65.988	1.00	20.00
ATOM	1812	SG	CYS	547	62.634	66.895	65.919	1.00	20.00
ATOM	1813	N	THR	548	64.765	70.309	67.067	1.00	20.00
ATOM	1814	CA	THR	548	66.007	70.179	67.764	1.00	20.00
ATOM	1815	C	THR	548	65.964	68.971	68.681	1.00	20.00
ATOM	1816	O	THR	548	66.935	68.114	68.684	1.00	20.00
ATOM	1817	CB	THR	548	66.227	71.286	68.793	1.00	20.00
ATOM	1818	OG1	THR	548	66.223	72.530	68.163	1.00	20.00
ATOM	1819	CG2	THR	548	67.582	71.015	69.470	1.00	20.00
ATOM	1820	N	GLY	549	64.808	68.565	69.096	1.00	20.00
ATOM	1821	CA	GLY	549	64.662	67.326	69.797	1.00	20.00
ATOM	1822	C	GLY	549	63.215	66.988	69.737	1.00	20.00
ATOM	1823	O	GLY	549	62.392	67.828	69.376	1.00	20.00
ATOM	1824	N	ARG	550	62.850	65.740	70.081	1.00	20.00
ATOM	1825	CA	ARG	550	61.455	65.449	70.004	1.00	20.00
ATOM	1826	C	ARG	550	60.772	66.258	71.052	1.00	20.00
ATOM	1827	O	ARG	550	61.294	66.467	72.146	1.00	20.00
ATOM	1828	CB	ARG	550	61.080	63.967	70.173	1.00	20.00
ATOM	1829	CG	ARG	550	61.455	63.132	68.947	1.00	20.00
ATOM	1830	CD	ARG	550	60.714	61.798	68.835	1.00	20.00
ATOM	1831	NE	ARG	550	61.225	60.888	69.897	1.00	20.00
ATOM	1832	CZ	ARG	550	60.590	59.702	70.129	1.00	20.00
ATOM	1833	NH1	ARG	550	59.473	59.377	69.414	1.00	20.00
ATOM	1834	NH2	ARG	550	61.072	58.842	71.073	1.00	20.00
ATOM	1835	N	GLY	551	59.575	66.762	70.706	1.00	20.00
ATOM	1836	CA	GLY	551	56.803	67.591	71.578	1.00	20.00
ATOM	1837	C	GLY	551	58.177	68.610	70.684	1.00	20.00
ATOM	1838	O	GLY	551	58.788	69.056	69.715	1.00	20.00
ATOM	1839	N	PRO	552	56.968	68.981	70.986	1.00	20.00
ATOM	1840	CA	PRO	552	56.283	69.935	70.152	1.00	20.00
ATOM	1841	C	PRO	552	56.820	71.333	70.250	1.00	20.00
ATOM	1842	O	PRO	552	56.470	72.163	69.411	1.00	20.00
ATOM	1843	CB	PRO	552	54.804	69.819	70.517	1.00	20.00
ATOM	1844	CG	PRO	552	54.662	68.367	71.004	1.00	20.00
ATOM	1845	CD	PRO	552	56.047	68.021	71.575	1.00	20.00
ATOM	1846	N	ASP	553	57.596	71.636	71.304	1.00	20.00
ATOM	1847	CA	ASP	553	58.187	72.933	71.507	1.00	20.00
ATOM	1848	C	ASP	553	59.368	73.115	70.593	1.00	20.00
ATOM	1849	O	ASP	553	59.695	74.227	70.184	1.00	20.00
ATOM	1850	CB	ASP	553	58.699	73.113	72.947	1.00	20.00
ATOM	1851	CG	ASP	553	59.092	74.568	73.163	1.00	20.00
ATOM	1852	OD1	ASP	553	58.823	75.401	72.258	1.00	20.00
ATOM	1853	OD2	ASP	553	59.672	74.864	74.242	1.00	20.00
ATOM	1854	N	ASN	554	60.057	72.005	70.285	1.00	20.00
ATOM	1855	CA	ASN	554	61.301	71.977	69.561	1.00	20.00
ATOM	1856	C	ASN	554	61.192	72.331	68.103	1.00	20.00
ATOM	1857	O	ASN	554	62.185	72.744	67.505	1.00	20.00
ATOM	1858	CB	ASN	554	62.017	70.621	69.675	1.00	20.00
ATOM	1859	CG	ASN	554	62.557	70.517	71.096	1.00	20.00
ATOM	1860	OD1	ASN	554	62.766	71.578	71.762	1.00	20.00
ATOM	1861	ND2	ASN	554	62.799	69.288	71.576	1.00	20.00
ATOM	1862	N	CYS	555	60.005	72.158	67.492	1.00	20.00
ATOM	1863	CA	CYS	555	59.774	72.307	66.076	1.00	20.00
ATOM	1864	C	CYS	555	60.501	73.479	65.475	1.00	20.00
ATOM	1865	O	CYS	555	60.788	74.475	66.138	1.00	20.00
ATOM	1866	CB	CYS	555	58.295	72.537	65.726	1.00	20.00
ATOM	1867	SG	CYS	555	57.153	71.342	66.479	1.00	20.00
ATOM	1868	N	ILE	556	60.926	73.314	64.200	1.00	20.00
ATOM	1869	CA	ILE	556	61.457	74.384	63.404	1.00	20.00
ATOM	1870	C	ILE	556	60.290	75.190	62.924	1.00	20.00
ATOM	1871	O	ILE	556	60.341	76.418	62.877	1.00	20.00
ATOM	1872	CB	ILE	556	62.242	73.888	62.210	1.00	20.00
ATOM	1873	CG1	ILE	556	62.951	75.036	61.457	1.00	20.00
ATOM	1874	CG2	ILE	556	61.312	73.038	61.328	1.00	20.00
ATOM	1875	CD1	ILE	556	62.039	76.016	60.716	1.00	20.00
ATOM	1876	N	GLN	557	59.210	74.481	62.533	1.00	20.00
ATOM	1877	CA	GLN	557	58.009	75.077	62.030	1.00	20.00
ATOM	1878	C	GLN	557	56.885	74.165	62.400	1.00	20.00
ATOM	1879	O	GLN	557	57.118	73.059	62.896	1.00	20.00
ATOM	1880	CB	GLN	557	57.980	75.245	60.502	1.00	20.00
ATOM	1881	CG	GLN	557	58.907	76.347	59.987	1.00	20.00
ATOM	1882	CD	GLN	557	58.316	77.684	60.415	1.00	20.00
ATOM	1883	OE1	GLN	557	59.218	77.983	61.604	1.00	20.00
ATOM	1884	NE2	GLN	557	57.905	78.513	59.418	1.00	20.00

Figure 6 (continued)

ATOM	1885	N	CYS	558	55.679	74.610	62.174	1.00	20.00
ATOM	1886	CA	CYS	558	54.500	73.819	62.573	1.00	20.00
ATOM	1887	C	CYS	558	53.790	73.313	61.357	1.00	20.00
ATOM	1888	O	CYS	558	53.817	73.939	60.300	1.00	20.00
ATOM	1889	CB	CYS	558	53.471	74.597	63.409	1.00	20.00
ATOM	1890	SG	CYS	558	54.165	75.235	64.962	1.00	20.00
ATOM	1891	N	ALA	559	53.193	72.110	61.491	1.00	20.00
ATOM	1892	CA	ALA	559	52.433	71.517	60.421	1.00	20.00
ATOM	1893	C	ALA	559	51.170	72.289	60.250	1.00	20.00
ATOM	1894	O	ALA	559	50.742	72.573	59.131	1.00	20.00
ATOM	1895	CB	ALA	559	52.047	70.085	60.721	1.00	20.00
ATOM	1896	N	HIS	560	50.557	72.673	61.384	1.00	20.00
ATOM	1897	CA	HIS	560	49.297	73.354	61.380	1.00	20.00
ATOM	1898	C	HIS	560	49.537	74.749	61.865	1.00	20.00
ATOM	1899	O	HIS	560	50.198	75.540	61.195	1.00	20.00
ATOM	1900	CB	HIS	560	48.260	72.703	62.312	1.00	20.00
ATOM	1901	CG	HIS	560	47.829	71.346	61.836	1.00	20.00
ATOM	1902	ND1	HIS	560	48.565	70.196	62.010	1.00	20.00
ATOM	1903	CD2	HIS	560	46.704	70.969	61.168	1.00	20.00
ATOM	1904	CE1	HIS	560	47.856	69.187	61.443	1.00	20.00
ATOM	1905	NE2	HIS	560	46.718	69.609	60.918	1.00	20.00
ATOM	1906	N	TYR	561	48.982	75.094	63.045	1.00	20.00
ATOM	1907	CA	TYR	561	49.080	76.446	63.536	1.00	20.00
ATOM	1908	C	TYR	561	49.975	76.468	64.736	1.00	20.00
ATOM	1909	O	TYR	561	49.968	75.545	65.548	1.00	20.00
ATOM	1910	CB	TYR	561	47.728	77.000	64.014	1.00	20.00
ATOM	1911	CG	TYR	561	46.778	76.861	62.878	1.00	20.00
ATOM	1912	CD1	TYR	561	46.145	75.658	62.667	1.00	20.00
ATOM	1913	CD2	TYR	561	46.518	77.912	62.029	1.00	20.00
ATOM	1914	CE1	TYR	561	45.264	75.499	61.624	1.00	20.00
ATOM	1915	CE2	TYR	561	45.637	77.759	60.984	1.00	20.00
ATOM	1916	CZ	TYR	561	45.010	76.553	60.780	1.00	20.00
ATOM	1917	OH	TYR	561	44.107	76.394	59.708	1.00	20.00
ATOM	1918	N	ILE	562	50.766	77.552	64.886	1.00	20.00
ATOM	1919	CA	ILE	562	51.630	77.640	66.027	1.00	20.00
ATOM	1920	C	ILE	562	50.986	78.554	67.021	1.00	20.00
ATOM	1921	O	ILE	562	50.464	79.608	66.661	1.00	20.00
ATOM	1922	CB	ILE	562	53.000	78.178	65.724	1.00	20.00
ATOM	1923	CG1	ILE	562	53.963	77.938	66.915	1.00	20.00
ATOM	1924	CG2	ILE	562	52.865	79.656	65.332	1.00	20.00
ATOM	1925	CD1	ILE	562	55.414	78.191	66.591	1.00	20.00
ATOM	1926	N	ASP	563	50.977	78.148	68.306	1.00	20.00
ATOM	1927	CA	ASP	563	50.359	78.961	69.312	1.00	20.00
ATOM	1928	C	ASP	563	51.118	78.619	70.593	1.00	20.00
ATOM	1929	O	ASP	563	51.329	77.697	71.049	1.00	20.00
ATOM	1930	CB	ASP	563	48.917	78.525	69.625	1.00	20.00
ATOM	1931	CG	ASP	563	48.364	79.426	70.722	1.00	20.00
ATOM	1932	OD1	ASP	563	48.956	80.511	70.959	1.00	20.00
ATOM	1933	OD2	ASP	563	47.343	79.032	71.348	1.00	20.00
ATOM	1934	N	GLY	564	51.509	79.966	71.206	1.00	20.00
ATOM	1935	CA	GLY	564	52.211	79.995	72.467	1.00	20.00
ATOM	1936	C	GLY	564	53.301	78.980	72.392	1.00	20.00
ATOM	1937	O	GLY	564	53.162	77.898	72.958	1.00	20.00
ATOM	1938	N	PRO	565	54.393	79.407	71.797	1.00	20.00
ATOM	1939	CA	PRO	565	55.444	78.525	71.327	1.00	20.00
ATOM	1940	C	PRO	565	56.183	77.051	71.369	1.00	20.00
ATOM	1941	O	PRO	565	56.038	76.285	71.810	1.00	20.00
ATOM	1942	CB	PRO	565	56.737	78.955	72.028	1.00	20.00
ATOM	1943	CG	PRO	565	56.299	80.027	73.038	1.00	20.00
ATOM	1944	CD	PRO	565	54.984	80.589	72.457	1.00	20.00
ATOM	1945	N	HIS	566	54.017	76.632	70.833	1.00	20.00
ATOM	1946	CA	HIS	566	53.669	75.240	70.771	1.00	20.00
ATOM	1947	C	HIS	566	53.069	75.013	69.432	1.00	20.00
ATOM	1948	O	HIS	566	52.273	75.826	68.964	1.00	20.00
ATOM	1949	CB	HIS	566	52.668	74.807	71.837	1.00	20.00
ATOM	1950	CG	HIS	566	52.550	73.319	71.982	1.00	20.00
ATOM	1951	ND1	HIS	566	53.361	72.562	72.797	1.00	20.00
ATOM	1952	CD2	HIS	566	51.688	72.444	71.397	1.00	20.00
ATOM	1953	CE1	HIS	566	52.953	71.274	72.668	1.00	20.00
ATOM	1954	NE2	HIS	566	51.940	71.153	71.829	1.00	20.00
ATOM	1955	N	CYS	567	53.417	73.895	68.765	1.00	20.00
ATOM	1956	CA	CYS	567	52.825	73.660	67.483	1.00	20.00
ATOM	1957	C	CYS	567	51.523	72.988	67.727	1.00	20.00
ATOM	1958	O	CYS	567	51.485	71.875	68.251	1.00	20.00
ATOM	1959	CB	CYS	567	53.639	72.751	66.551	1.00	20.00
ATOM	1960	SG	CYS	567	55.046	73.611	65.799	1.00	20.00
ATOM	1961	N	VAL	568	50.416	73.689	67.340	1.00	20.00

Figure 6 (continued)

ATOM	1962	CA	VAL	568	49.128	73.100	67.619	1.00 20.00
ATOM	1963	C	VAL	568	48.478	72.735	66.317	1.00 20.00
ATOM	1964	O	VAL	568	48.734	73.341	65.276	1.00 20.00
ATOM	1965	CB	VAL	568	48.227	74.019	68.361	1.00 20.00
ATOM	1966	CG1	VAL	568	46.905	73.276	68.601	1.00 20.00
ATOM	1967	CG2	VAL	568	48.932	74.455	69.676	1.00 20.00
ATOM	1968	N	LYS	569	47.655	71.664	66.351	1.00 20.00
ATOM	1969	CA	LYS	569	46.930	71.150	65.220	1.00 20.00
ATOM	1970	C	LYS	569	45.838	72.095	64.828	1.00 20.00
ATOM	1971	O	LYS	569	45.511	72.223	63.648	1.00 20.00
ATOM	1972	CB	LYS	569	46.257	69.797	65.513	1.00 20.00
ATOM	1973	CG	LYS	569	45.478	69.230	64.323	1.00 20.00
ATOM	1974	CD	LYS	569	45.008	67.788	64.523	1.00 20.00
ATOM	1975	CE	LYS	569	44.141	67.257	63.377	1.00 20.00
ATOM	1976	NZ	LYS	569	43.723	65.865	63.661	1.00 20.00
ATOM	1977	N	THR	570	45.197	72.738	65.823	1.00 20.00
ATOM	1978	CA	THR	570	44.134	73.648	65.517	1.00 20.00
ATOM	1979	C	THR	570	44.127	74.693	66.581	1.00 20.00
ATOM	1980	O	THR	570	44.661	74.502	67.668	1.00 20.00
ATOM	1981	CB	THR	570	42.779	73.003	65.508	1.00 20.00
ATOM	1982	OG1	THR	570	42.471	72.494	66.798	1.00 20.00
ATOM	1983	CG2	THR	570	42.782	71.864	64.475	1.00 20.00
ATOM	1984	N	CYS	571	43.504	75.843	66.293	1.00 20.00
ATOM	1985	CA	CYS	571	43.476	76.920	67.234	1.00 20.00
ATOM	1986	C	CYS	571	42.741	76.506	68.472	1.00 20.00
ATOM	1987	O	CYS	571	41.757	75.772	68.441	1.00 20.00
ATOM	1988	CB	CYS	571	42.716	78.132	66.691	1.00 20.00
ATOM	1989	SG	CYS	571	43.685	79.164	65.569	1.00 20.00
ATOM	1990	N	PRO	572	43.236	77.006	69.573	1.00 20.00
ATOM	1991	CA	PRO	572	42.619	76.786	70.856	1.00 20.00
ATOM	1992	C	PRO	572	41.430	77.693	70.943	1.00 20.00
ATOM	1993	O	PRO	572	41.348	78.636	70.160	1.00 20.00
ATOM	1994	CB	PRO	572	43.697	77.075	71.902	1.00 20.00
ATOM	1995	CG	PRO	572	44.798	77.823	71.132	1.00 20.00
ATOM	1996	CD	PRO	572	44.649	77.315	69.690	1.00 20.00
ATOM	1997	N	ALA	573	40.498	77.433	71.881	1.00 20.00
ATOM	1998	CA	ALA	573	39.307	78.232	71.961	1.00 20.00
ATOM	1999	C	ALA	573	39.668	79.625	72.367	1.00 20.00
ATOM	2000	O	ALA	573	40.596	78.845	73.141	1.00 20.00
ATOM	2001	CB	ALA	573	38.277	77.700	72.974	1.00 20.00
ATOM	2002	N	GLY	574	38.937	80.611	71.805	1.00 20.00
ATOM	2003	CA	GLY	574	39.109	81.993	72.150	1.00 20.00
ATOM	2004	C	GLY	574	40.195	82.578	71.310	1.00 20.00
ATOM	2005	O	GLY	574	40.421	83.788	71.337	1.00 20.00
ATOM	2006	N	VAL	575	40.903	81.741	70.531	1.00 20.00
ATOM	2007	CA	VAL	575	41.961	82.289	69.736	1.00 20.00
ATOM	2008	C	VAL	575	41.649	81.875	68.326	1.00 20.00
ATOM	2009	O	VAL	575	41.123	80.787	68.100	1.00 20.00
ATOM	2010	CB	VAL	575	43.302	81.755	70.258	1.00 20.00
ATOM	2011	CG1	VAL	575	44.403	82.365	69.385	1.00 20.00
ATOM	2012	CG2	VAL	575	43.480	82.030	71.660	1.00 20.00
ATOM	2013	N	MET	576	41.928	82.748	67.334	1.00 20.00
ATOM	2014	CA	MET	576	41.683	82.424	65.978	1.00 20.00
ATOM	2015	C	MET	576	42.802	82.464	65.123	1.00 20.00
ATOM	2016	O	MET	576	43.766	83.166	65.416	1.00 20.00
ATOM	2017	CB	MET	576	40.656	83.382	65.350	1.00 20.00
ATOM	2018	CG	MET	576	40.195	83.020	63.907	1.00 20.00
ATOM	2019	SD	MET	576	38.885	84.064	63.171	1.00 20.00
ATOM	2020	CE	MET	576	37.528	83.226	64.039	1.00 20.00
ATOM	2021	N	GLY	577	42.786	81.678	64.030	1.00 20.00
ATOM	2022	CA	GLY	577	43.921	81.593	63.165	1.00 20.00
ATOM	2023	C	GLY	577	44.090	82.900	62.474	1.00 20.00
ATOM	2024	O	GLY	577	43.127	83.494	61.989	1.00 20.00
ATOM	2025	N	GLU	578	45.343	83.379	62.371	1.00 40.00
ATOM	2026	CA	GLU	578	45.547	84.629	61.705	1.00 40.00
ATOM	2027	C	GLU	578	45.290	84.395	60.256	1.00 40.00
ATOM	2028	O	GLU	578	45.577	83.321	59.729	1.00 40.00
ATOM	2029	CB	GLU	578	46.973	85.187	61.850	1.00 40.00
ATOM	2030	CG	GLU	578	47.160	86.558	61.196	1.00 40.00
ATOM	2031	CD	GLU	578	48.604	86.987	61.414	1.00 40.00
ATOM	2032	OE1	GLU	578	49.512	86.143	61.187	1.00 40.00
ATOM	2033	OE2	GLU	578	48.818	88.167	61.816	1.00 40.00
ATOM	2034	N	ASN	579	44.716	85.402	59.571	1.00 60.00
ATOM	2035	CA	ASN	579	44.440	85.235	58.178	1.00 60.00
ATOM	2036	C	ASN	579	45.210	86.275	57.439	1.00 60.00
ATOM	2037	O	ASN	579	45.442	87.373	57.943	1.00 60.00
ATOM	2038	CB	ASN	579	42.958	85.427	57.811	1.00 60.00

Figure 6 (continued)

ATOM	2039	CG	ASN	579	42.172	84.264	58.397	1.00	60.00
ATOM	2040	OD1	ASN	579	42.728	83.211	58.705	1.00	60.00
ATOM	2041	ND2	ASN	579	40.834	84.454	58.548	1.00	60.00
ATOM	2042	N	ASN	580	45.637	85.936	56.210	1.00	60.00
ATOM	2043	CA	ASN	580	46.365	86.867	55.405	1.00	60.00
ATOM	2044	C	ASN	580	45.562	87.066	54.165	1.00	60.00
ATOM	2045	O	ASN	580	44.794	86.193	53.764	1.00	60.00
ATOM	2046	CB	ASN	580	47.759	86.367	54.990	1.00	60.00
ATOM	2047	CG	ASN	580	48.640	86.362	56.231	1.00	60.00
ATOM	2048	OD1	ASN	580	48.848	87.397	56.864	1.00	60.00
ATOM	2049	ND2	ASN	580	49.170	85.165	56.599	1.00	60.00
ATOM	2050	N	THR	581	45.706	88.244	53.532	1.00	60.00
ATOM	2051	CA	THR	581	44.944	88.510	52.352	1.00	60.00
ATOM	2052	C	THR	581	45.336	87.507	51.321	1.00	60.00
ATOM	2053	O	THR	581	44.483	86.912	50.665	1.00	60.00
ATOM	2054	CB	THR	581	45.206	89.875	51.789	1.00	60.00
ATOM	2055	OG1	THR	581	46.569	90.000	51.416	1.00	60.00
ATOM	2056	CG2	THR	581	44.852	90.922	52.860	1.00	60.00
ATOM	2057	N	LEU	582	46.653	87.277	51.164	1.00	60.00
ATOM	2058	CA	LEU	582	47.091	86.320	50.194	1.00	60.00
ATOM	2059	C	LEU	582	46.855	84.968	50.770	1.00	60.00
ATOM	2060	O	LEU	582	46.752	84.807	51.986	1.00	60.00
ATOM	2061	CB	LEU	582	48.588	86.413	49.847	1.00	60.00
ATOM	2062	CG	LEU	582	48.995	87.727	49.151	1.00	60.00
ATOM	2063	CD1	LEU	582	48.324	87.865	47.776	1.00	60.00
ATOM	2064	CD2	LEU	582	48.762	88.942	50.062	1.00	60.00
ATOM	2065	N	VAL	583	46.742	83.951	49.896	1.00	60.00
ATOM	2066	CA	VAL	583	46.540	82.620	50.376	1.00	60.00
ATOM	2067	C	VAL	583	47.867	81.945	50.317	1.00	60.00
ATOM	2068	O	VAL	583	48.581	82.039	49.319	1.00	60.00
ATOM	2069	CB	VAL	583	45.575	81.819	49.550	1.00	60.00
ATOM	2070	CG1	VAL	583	46.137	81.681	48.124	1.00	60.00
ATOM	2071	CG2	VAL	583	45.334	80.474	50.254	1.00	60.00
ATOM	2072	N	TRP	584	48.250	81.263	51.412	1.00	60.00
ATOM	2073	CA	TRP	584	49.530	80.628	51.419	1.00	60.00
ATOM	2074	C	TRP	584	49.379	79.268	50.829	1.00	60.00
ATOM	2075	O	TRP	584	48.336	78.624	50.967	1.00	60.00
ATOM	2076	CB	TRP	584	50.140	80.483	52.819	1.00	60.00
ATOM	2077	CG	TRP	584	50.459	81.808	53.468	1.00	60.00
ATOM	2078	CD1	TRP	584	49.828	82.439	54.500	1.00	60.00
ATOM	2079	CD2	TRP	584	51.521	82.679	53.047	1.00	60.00
ATOM	2080	NE1	TRP	584	50.435	83.646	54.753	1.00	60.00
ATOM	2081	CE2	TRP	584	51.476	83.808	53.865	1.00	60.00
ATOM	2082	CE3	TRP	584	52.453	82.581	52.058	1.00	60.00
ATOM	2083	CZ2	TRP	584	52.368	84.830	53.706	1.00	60.00
ATOM	2084	CZ3	TRP	584	53.353	83.587	51.903	1.00	60.00
ATOM	2085	CH2	TRP	584	53.311	84.699	52.710	1.00	60.00
ATOM	2086	N	LYS	585	50.430	78.812	50.126	1.00	60.00
ATOM	2087	CA	LYS	585	50.401	77.536	49.481	1.00	60.00
ATOM	2088	C	LYS	585	50.330	76.447	50.502	1.00	60.00
ATOM	2089	O	LYS	585	49.644	75.513	50.356	1.00	60.00
ATOM	2090	CB	LYS	585	51.648	77.271	48.620	1.00	60.00
ATOM	2091	CG	LYS	585	51.717	78.119	47.347	1.00	60.00
ATOM	2092	CD	LYS	585	50.561	77.861	46.378	1.00	60.00
ATOM	2093	CE	LYS	585	50.624	78.707	45.105	1.00	60.00
ATOM	2094	NZ	LYS	585	50.489	80.141	45.444	1.00	60.00
ATOM	2095	N	TYR	586	51.139	76.529	51.577	1.00	60.00
ATOM	2096	CA	TYR	586	51.131	75.431	52.473	1.00	60.00
ATOM	2097	C	TYR	586	51.541	75.835	53.848	1.00	60.00
ATOM	2098	O	TYR	586	51.345	76.975	54.267	1.00	60.00
ATOM	2099	CB	TYR	586	52.101	74.294	52.050	1.00	60.00
ATOM	2100	CG	TYR	586	51.639	73.778	50.731	1.00	60.00
ATOM	2101	CD1	TYR	586	50.620	72.855	50.658	1.00	60.00
ATOM	2102	CD2	TYR	586	52.227	74.214	49.565	1.00	60.00
ATOM	2103	CE1	TYR	586	50.192	72.378	49.442	1.00	60.00
ATOM	2104	CE2	TYR	586	51.804	73.741	48.346	1.00	60.00
ATOM	2105	CZ	TYR	586	50.784	72.822	48.283	1.00	60.00
ATOM	2106	OH	TYR	586	50.347	72.333	47.033	1.00	60.00
ATOM	2107	N	ALA	587	52.121	74.860	54.576	1.00	60.00
ATOM	2108	CA	ALA	587	52.573	74.951	55.933	1.00	60.00
ATOM	2109	C	ALA	587	53.640	75.987	56.000	1.00	60.00
ATOM	2110	O	ALA	587	53.895	76.560	57.057	1.00	60.00
ATOM	2111	CB	ALA	587	53.162	73.631	56.484	1.00	60.00
ATOM	2112	N	ASP	588	54.295	76.249	54.857	1.00	60.00
ATOM	2113	CA	ASP	588	55.364	77.220	54.795	1.00	60.00
ATOM	2114	C	ASP	588	54.762	78.493	55.316	1.00	60.00
ATOM	2115	O	ASP	588	55.465	79.320	55.896	1.00	60.00

Figure 6 (continued)

ATOM	2116	CB	ASP	588	55.828	77.482	53.358	1.00	60.00
ATOM	2117	CG	ASP	588	56.540	76.233	52.853	1.00	60.00
ATOM	2118	OD1	ASP	588	56.754	75.301	53.675	1.00	60.00
ATOM	2119	OD2	ASP	588	56.872	76.190	51.639	1.00	60.00
ATOM	2120	N	ALA	589	53.442	78.671	55.134	1.00	60.00
ATOM	2121	CA	ALA	589	52.783	79.858	55.590	1.00	60.00
ATOM	2122	C	ALA	589	53.064	80.002	57.080	1.00	60.00
ATOM	2123	O	ALA	589	53.375	81.096	57.519	1.00	60.00
ATOM	2124	CB	ALA	589	51.255	79.775	55.450	1.00	60.00
ATOM	2125	N	GLY	590	52.983	78.897	57.812	1.00	60.00
ATOM	2126	CA	GLY	590	53.267	79.002	59.213	1.00	60.00
ATOM	2127	C	GLY	590	52.138	79.727	59.867	1.00	60.00
ATOM	2128	O	GLY	590	52.347	80.690	60.605	1.00	60.00
ATOM	2129	N	HIS	591	50.899	79.280	59.599	1.00	60.00
ATOM	2130	CA	HIS	591	49.751	79.919	60.168	1.00	60.00
ATOM	2131	C	HIS	591	49.902	79.896	61.655	1.00	60.00
ATOM	2132	O	HIS	591	50.347	78.909	62.237	1.00	60.00
ATOM	2133	CB	HIS	591	48.433	79.207	59.822	1.00	60.00
ATOM	2134	CG	HIS	591	48.187	79.120	58.346	1.00	60.00
ATOM	2135	ND1	HIS	591	48.714	78.152	57.529	1.00	60.00
ATOM	2136	CD2	HIS	591	47.455	79.938	57.532	1.00	60.00
ATOM	2137	CE1	HIS	591	48.277	78.415	56.272	1.00	60.00
ATOM	2138	NE2	HIS	591	47.509	79.490	56.224	1.00	60.00
ATOM	2139	N	VAL	592	49.535	81.017	62.305	1.00	40.00
ATOM	2140	CA	VAL	592	49.640	81.132	63.730	1.00	40.00
ATOM	2141	C	VAL	592	48.276	81.467	64.234	1.00	40.00
ATOM	2142	O	VAL	592	47.414	81.895	63.467	1.00	40.00
ATOM	2143	CB	VAL	592	50.554	82.238	64.164	1.00	40.00
ATOM	2144	CG1	VAL	592	51.975	81.924	63.670	1.00	40.00
ATOM	2145	CG2	VAL	592	49.999	83.563	63.620	1.00	40.00
ATOM	2146	N	CYS	593	48.030	81.264	65.544	1.00	20.00
ATOM	2147	CA	CYS	593	46.725	81.565	66.036	1.00	20.00
ATOM	2148	C	CYS	593	46.060	82.778	66.911	1.00	20.00
ATOM	2149	O	CYS	593	47.823	82.899	67.666	1.00	20.00
ATOM	2150	CB	CYS	593	46.131	80.416	66.864	1.00	20.00
ATOM	2151	SG	CYS	593	44.332	80.552	66.886	1.00	20.00
ATOM	2152	N	HIS	594	45.905	83.729	66.811	1.00	20.00
ATOM	2153	CA	HIS	594	45.983	84.931	67.595	1.00	20.00
ATOM	2154	C	HIS	594	44.693	85.136	68.325	1.00	20.00
ATOM	2155	O	HIS	594	43.649	84.625	67.926	1.00	20.00
ATOM	2156	CB	HIS	594	46.256	86.197	66.765	1.00	20.00
ATOM	2157	CG	HIS	594	47.645	86.226	66.200	1.00	20.00
ATOM	2158	ND1	HIS	594	48.743	86.699	66.887	1.00	20.00
ATOM	2159	CD2	HIS	594	48.109	85.821	64.986	1.00	20.00
ATOM	2160	CE1	HIS	594	49.808	86.558	66.054	1.00	20.00
ATOM	2161	NE2	HIS	594	49.473	86.031	64.892	1.00	20.00
ATOM	2162	N	LEU	595	44.747	85.910	69.426	1.00	20.00
ATOM	2163	CA	LEU	595	43.613	86.140	70.276	1.00	20.00
ATOM	2164	C	LEU	595	42.596	86.943	69.557	1.00	20.00
ATOM	2165	O	LEU	595	42.911	87.735	68.669	1.00	20.00
ATOM	2166	CB	LEU	595	43.970	86.903	71.565	1.00	20.00
ATOM	2167	CG	LEU	595	44.979	86.165	72.460	1.00	20.00
ATOM	2168	CD1	LEU	595	45.296	86.970	73.730	1.00	20.00
ATOM	2169	CD2	LEU	595	44.522	84.731	72.758	1.00	20.00
ATOM	2170	N	CYS	596	41.319	86.724	69.922	1.00	20.00
ATOM	2171	CA	CYS	596	40.264	87.490	69.344	1.00	20.00
ATOM	2172	C	CYS	596	39.852	88.447	70.418	1.00	20.00
ATOM	2173	O	CYS	596	39.751	88.078	71.586	1.00	20.00
ATOM	2174	CB	CYS	596	39.065	86.636	68.890	1.00	20.00
ATOM	2175	SG	CYS	596	37.811	87.561	67.948	1.00	20.00
ATOM	2176	N	HIS	597	39.630	89.722	70.048	1.00	20.00
ATOM	2177	CA	HIS	597	39.306	90.720	71.027	1.00	20.00
ATOM	2178	C	HIS	597	37.999	90.354	71.647	1.00	20.00
ATOM	2179	O	HIS	597	37.160	89.701	71.033	1.00	20.00
ATOM	2180	CB	HIS	597	39.201	92.134	70.430	1.00	20.00
ATOM	2181	CG	HIS	597	38.981	93.202	71.456	1.00	20.00
ATOM	2182	ND1	HIS	597	39.845	93.457	72.497	1.00	20.00
ATOM	2183	CD2	HIS	597	37.971	94.104	71.583	1.00	20.00
ATOM	2184	CE1	HIS	597	39.319	94.493	73.196	1.00	20.00
ATOM	2185	NE2	HIS	597	38.181	94.920	72.680	1.00	20.00
ATOM	2186	N	PRO	598	37.823	90.734	72.880	1.00	20.00
ATOM	2187	CA	PRO	598	36.602	90.420	73.560	1.00	20.00
ATOM	2188	C	PRO	598	35.445	91.195	73.019	1.00	20.00
ATOM	2189	O	PRO	598	34.314	90.732	73.154	1.00	20.00
ATOM	2190	CB	PRO	598	36.875	90.632	75.052	1.00	20.00
ATOM	2191	CG	PRO	598	38.248	91.329	75.109	1.00	20.00
ATOM	2192	CD	PRO	598	38.932	90.896	73.803	1.00	20.00

Figure 6 (continued)

ATOM	2193	N	ASN	599	35.692	92.390	72.448	1.00	20.00
ATOM	2194	CA	ASN	599	34.620	93.172	71.902	1.00	20.00
ATOM	2195	C	ASN	599	34.122	92.537	70.643	1.00	20.00
ATOM	2196	O	ASN	599	32.917	92.417	70.434	1.00	20.00
ATOM	2197	CB	ASN	599	35.028	94.615	71.556	1.00	20.00
ATOM	2198	CG	ASN	599	35.318	95.347	72.859	1.00	20.00
ATOM	2199	OD1	ASN	599	34.984	94.867	73.942	1.00	20.00
ATOM	2200	ND2	ASN	599	35.951	96.546	72.755	1.00	20.00
ATOM	2201	N	CYS	600	35.043	92.082	69.771	1.00	20.00
ATOM	2202	CA	CYS	600	34.608	91.561	68.509	1.00	20.00
ATOM	2203	C	CYS	600	33.767	90.362	68.773	1.00	20.00
ATOM	2204	O	CYS	600	33.836	89.762	69.845	1.00	20.00
ATOM	2205	CB	CYS	600	35.743	91.107	67.573	1.00	20.00
ATOM	2206	SG	CYS	600	36.923	92.422	67.157	1.00	20.00
ATOM	2207	N	THR	601	32.911	90.007	67.797	1.00	20.00
ATOM	2208	CA	THR	601	32.099	88.846	67.972	1.00	20.00
ATOM	2209	C	THR	601	32.181	88.032	66.721	1.00	20.00
ATOM	2210	O	THR	601	32.335	88.561	65.620	1.00	20.00
ATOM	2211	CB	THR	601	30.652	89.158	68.217	1.00	20.00
ATOM	2212	OG1	THR	601	30.095	89.826	67.095	1.00	20.00
ATOM	2213	CG2	THR	601	30.549	90.046	69.469	1.00	20.00
ATOM	2214	N	TYR	602	32.100	86.700	66.886	1.00	20.00
ATOM	2215	CA	TYR	602	32.070	85.753	65.812	1.00	20.00
ATOM	2216	C	TYR	602	33.273	85.827	64.922	1.00	20.00
ATOM	2217	O	TYR	602	33.163	85.523	63.737	1.00	20.00
ATOM	2218	CB	TYR	602	30.813	85.876	64.933	1.00	20.00
ATOM	2219	CG	TYR	602	29.647	85.457	65.761	1.00	20.00
ATOM	2220	CD1	TYR	602	29.350	84.122	65.912	1.00	20.00
ATOM	2221	CD2	TYR	602	28.851	86.390	66.383	1.00	20.00
ATOM	2222	CE1	TYR	602	28.277	83.722	66.672	1.00	20.00
ATOM	2223	CE2	TYR	602	27.775	85.987	67.145	1.00	20.00
ATOM	2224	CZ	TYR	602	27.488	84.660	67.289	1.00	20.00
ATOM	2225	OH	TYR	602	26.385	84.253	68.070	1.00	20.00
ATOM	2226	N	GLY	603	34.459	86.213	65.434	1.00	20.00
ATOM	2227	CA	GLY	603	35.588	86.115	64.549	1.00	20.00
ATOM	2228	C	GLY	603	36.486	87.304	64.674	1.00	20.00
ATOM	2229	O	GLY	603	36.071	88.380	65.101	1.00	20.00
ATOM	2230	N	CYS	604	37.769	87.113	64.288	1.00	20.00
ATOM	2231	CA	CYS	604	38.732	88.176	64.298	1.00	20.00
ATOM	2232	C	CYS	604	39.680	87.981	63.155	1.00	20.00
ATOM	2233	O	CYS	604	40.163	86.875	62.911	1.00	20.00
ATOM	2234	CB	CYS	604	39.519	88.219	65.588	1.00	20.00
ATOM	2235	SG	CYS	604	38.876	89.016	67.014	1.00	20.00
ATOM	2236	N	THR	605	39.943	89.064	62.398	1.00	20.00
ATOM	2237	CA	THR	605	40.928	89.017	61.358	1.00	20.00
ATOM	2238	C	THR	605	42.250	88.915	62.047	1.00	20.00
ATOM	2239	O	THR	605	43.123	88.142	61.654	1.00	20.00
ATOM	2240	CB	THR	605	40.941	90.260	60.520	1.00	20.00
ATOM	2241	OG1	THR	605	41.253	91.390	61.322	1.00	20.00
ATOM	2242	CG2	THR	605	39.556	90.431	59.874	1.00	20.00
ATOM	2243	N	GLY	606	42.403	89.706	63.126	1.00	20.00
ATOM	2244	CA	GLY	606	43.605	89.745	63.903	1.00	20.00
ATOM	2245	C	GLY	606	43.221	90.378	65.198	1.00	20.00
ATOM	2246	O	GLY	606	42.042	90.614	65.456	1.00	20.00
ATOM	2247	N	PRO	607	44.177	90.654	66.036	1.00	20.00
ATOM	2248	CA	PRO	607	43.861	91.278	67.288	1.00	20.00
ATOM	2249	C	PRO	607	43.557	92.720	67.061	1.00	20.00
ATOM	2250	O	PRO	607	44.089	93.297	66.113	1.00	20.00
ATOM	2251	CB	PRO	607	45.058	91.074	68.209	1.00	20.00
ATOM	2252	CG	PRO	607	46.162	90.484	67.279	1.00	20.00
ATOM	2253	CD	PRO	607	45.383	89.851	66.116	1.00	20.00
ATOM	2254	N	GLY	608	42.698	93.320	67.908	1.00	20.00
ATOM	2255	CA	GLY	608	42.388	94.708	67.751	1.00	20.00
ATOM	2256	C	GLY	608	40.920	94.842	67.505	1.00	20.00
ATOM	2257	O	GLY	608	40.263	93.913	67.037	1.00	20.00
ATOM	2258	N	LEU	609	40.378	96.033	67.826	1.00	20.00
ATOM	2259	CA	LEU	609	38.991	96.344	67.647	1.00	20.00
ATOM	2260	C	LEU	609	38.726	96.337	66.177	1.00	20.00
ATOM	2261	O	LEU	609	37.661	95.926	65.719	1.00	20.00
ATOM	2262	CB	LEU	609	38.635	97.750	68.158	1.00	20.00
ATOM	2263	CG	LEU	609	38.904	97.960	69.660	1.00	20.00
ATOM	2264	CD1	LEU	609	40.404	97.860	69.978	1.00	20.00
ATOM	2265	CD2	LEU	609	38.271	99.269	70.161	1.00	20.00
ATOM	2266	N	GLU	610	39.720	96.803	65.404	1.00	20.00
ATOM	2267	CA	GLU	610	39.640	96.911	63.976	1.00	20.00
ATOM	2268	C	GLU	610	39.475	95.539	63.422	1.00	20.00
ATOM	2269	O	GLU	610	38.824	95.343	62.396	1.00	20.00

Figure 6 (continued)

ATOM	2270	CB	GLU	610	40.943	97.471	63.365	1.00	20.00
ATOM	2271	CG	GLU	610	41.251	98.915	63.761	1.00	20.00
ATOM	2272	CD	GLU	610	42.556	99.307	63.078	1.00	20.00
ATOM	2273	OE1	GLU	610	42.743	98.912	61.897	1.00	20.00
ATOM	2274	OE2	GLU	610	43.380	100.002	63.731	1.00	20.00
ATOM	2275	N	GLY	611	40.055	94.569	64.118	1.00	20.00
ATOM	2276	CA	GLY	611	40.073	93.186	63.684	1.00	20.00
ATOM	2277	C	GLY	611	38.677	92.696	63.492	1.00	20.00
ATOM	2278	O	GLY	611	38.460	91.787	62.690	1.00	20.00
ATOM	2279	N	CYS	612	37.717	93.255	64.254	1.00	20.00
ATOM	2280	CA	CYS	612	36.359	92.832	64.099	1.00	20.00
ATOM	2281	C	CYS	612	36.021	93.691	62.670	1.00	20.00
ATOM	2282	O	CYS	612	36.613	93.962	62.033	1.00	20.00
ATOM	2283	CB	CYS	612	35.328	93.660	64.892	1.00	20.00
ATOM	2284	SG	CYS	612	35.756	93.986	66.626	1.00	20.00
ATOM	2285	N	PRO	613	35.097	92.336	62.146	1.00	60.00
ATOM	2286	CA	PRO	613	34.670	92.528	60.790	1.00	60.00
ATOM	2287	C	PRO	613	34.223	93.951	60.698	1.00	60.00
ATOM	2288	O	PRO	613	33.656	94.455	61.666	1.00	60.00
ATOM	2289	CB	PRO	613	33.493	91.578	60.603	1.00	60.00
ATOM	2290	CG	PRO	613	32.874	91.515	62.012	1.00	60.00
ATOM	2291	CD	PRO	613	34.079	91.688	62.955	1.00	60.00
ATOM	2292	N	THR	614	34.478	94.629	59.564	1.00	60.00
ATOM	2293	CA	THR	614	34.088	95.997	59.486	1.00	60.00
ATOM	2294	C	THR	614	33.136	96.141	58.331	1.00	60.00
ATOM	2295	O	THR	614	33.362	95.585	57.258	1.00	60.00
ATOM	2296	CB	THR	614	35.205	96.950	59.259	1.00	60.00
ATOM	2297	OG1	THR	614	36.143	96.856	60.322	1.00	60.00
ATOM	2298	OG2	THR	614	34.639	98.370	59.179	1.00	60.00
ATOM	2299	N	ASN	615	32.040	96.892	58.544	1.00	60.00
ATOM	2300	CA	ASN	615	31.101	97.135	57.494	1.00	60.00
ATOM	2301	C	ASN	615	31.794	97.963	56.478	1.00	60.00
ATOM	2302	O	ASN	615	31.612	97.805	55.275	1.00	60.00
ATOM	2303	CB	ASN	615	29.831	97.862	57.973	1.00	60.00
ATOM	2304	CG	ASN	615	30.226	99.212	58.581	1.00	60.00
ATOM	2305	OD1	ASN	615	31.259	99.344	59.205	1.00	60.00
ATOM	2306	ND2	ASN	615	29.374	100.243	58.309	1.00	60.00
ATOM	2307	N	GLY	616	32.636	98.921	56.953	1.00	60.00
ATOM	2308	CA	GLY	616	33.362	99.779	56.061	1.00	60.00
ATOM	2309	C	GLY	616	32.429	100.789	55.469	1.00	60.00
ATOM	2310	O	GLY	616	32.488	101.080	54.270	1.00	60.00
ATOM	2311	N	PRO	617	31.571	101.360	56.274	1.00	60.00
ATOM	2312	CA	PRO	617	30.612	102.308	55.777	1.00	60.00
ATOM	2313	C	PRO	617	31.360	103.413	55.104	1.00	60.00
ATOM	2314	O	PRO	617	32.523	103.636	55.437	1.00	60.00
ATOM	2315	CB	PRO	617	29.906	102.846	57.013	1.00	60.00
ATOM	2316	CG	PRO	617	31.027	102.833	58.067	1.00	60.00
ATOM	2317	CD	PRO	617	31.897	101.629	57.667	1.00	60.00
ATOM	2318	N	LYS	618	30.717	104.103	54.145	1.00	60.00
ATOM	2319	CA	LYS	618	31.363	105.196	53.470	1.00	60.00
ATOM	2320	C	LYS	618	31.672	106.227	54.494	1.00	60.00
ATOM	2321	O	LYS	618	32.768	106.782	54.517	1.00	60.00
ATOM	2322	CB	LYS	618	30.470	105.844	52.405	1.00	60.00
ATOM	2323	CG	LYS	618	30.300	105.010	51.134	1.00	60.00
ATOM	2324	CD	LYS	618	31.607	104.810	50.364	1.00	60.00
ATOM	2325	CE	LYS	618	31.453	103.977	49.091	1.00	60.00
ATOM	2326	NZ	LYS	618	32.740	103.929	48.362	1.00	60.00
ATOM	2327	N	ILE	619	30.705	106.503	55.389	1.00	60.00
ATOM	2328	CA	ILE	619	30.930	107.501	56.390	1.00	60.00
ATOM	2329	C	ILE	619	32.013	107.002	57.281	1.00	60.00
ATOM	2330	O	ILE	619	32.155	105.803	57.518	1.00	60.00
ATOM	2331	CB	ILE	619	29.732	107.775	57.253	1.00	60.00
ATOM	2332	CG1	ILE	619	28.558	108.285	56.401	1.00	60.00
ATOM	2333	CG2	ILE	619	30.164	108.744	58.365	1.00	60.00
ATOM	2334	CD1	ILE	619	28.868	109.573	55.641	1.00	60.00
ATOM	2335	N	PRO	620	32.809	107.922	57.744	1.00	60.00
ATOM	2336	CA	PRO	620	33.873	107.585	58.644	1.00	60.00
ATOM	2337	C	PRO	620	33.318	107.382	60.013	1.00	60.00
ATOM	2338	O	PRO	620	32.243	107.904	60.304	1.00	60.00
ATOM	2339	CB	PRO	620	34.892	108.725	58.549	1.00	60.00
ATOM	2340	CG	PRO	620	34.143	109.860	57.827	1.00	60.00
ATOM	2341	CD	PRO	620	33.099	109.120	56.978	1.00	60.00
ATOM	2342	N	SER	621	34.027	106.617	60.864	1.00	60.00
ATOM	2343	CA	SER	621	33.548	106.395	62.193	1.00	60.00
ATOM	2344	C	SER	621	33.775	107.684	62.974	1.00	60.00
ATOM	2345	O	SER	621	33.285	108.746	62.511	1.00	60.00
ATOM	2346	CB	SER	621	34.281	105.252	62.921	1.00	60.00

Figure 6 (continued)

```
ATOM   2347  OG  SER   621      35.659 105.566  63.074  1.00 60.00
ATOM   2348  OXT SER   621      34.446 107.626  64.041  1.00 60.00
TER
```

Figure 6 (continued)

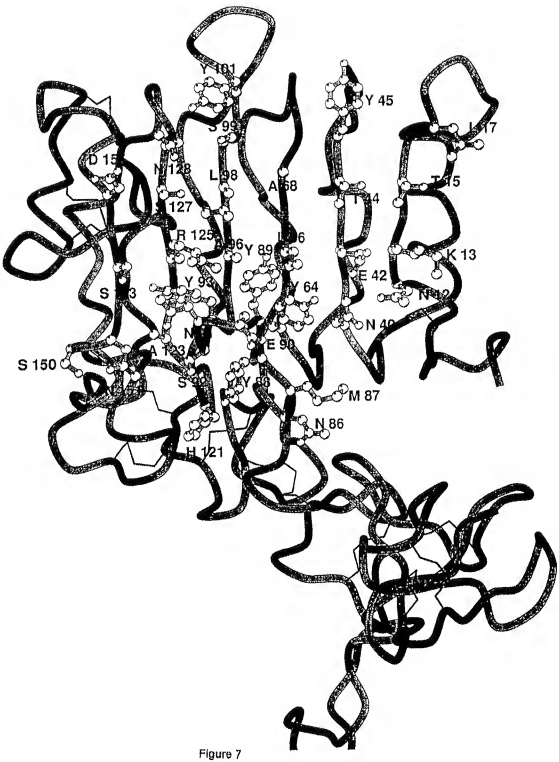

Figure 7

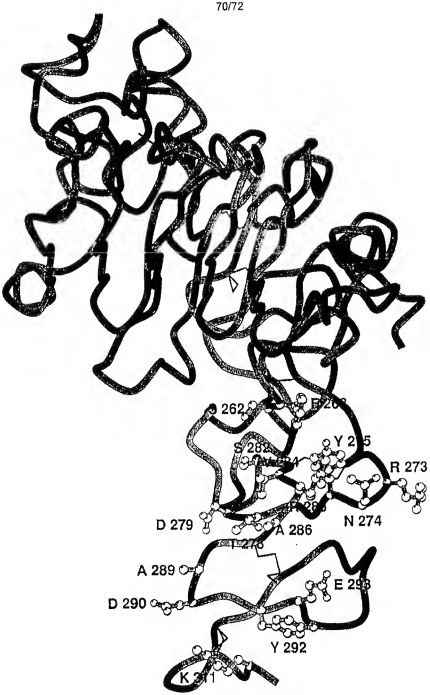

Figure 8

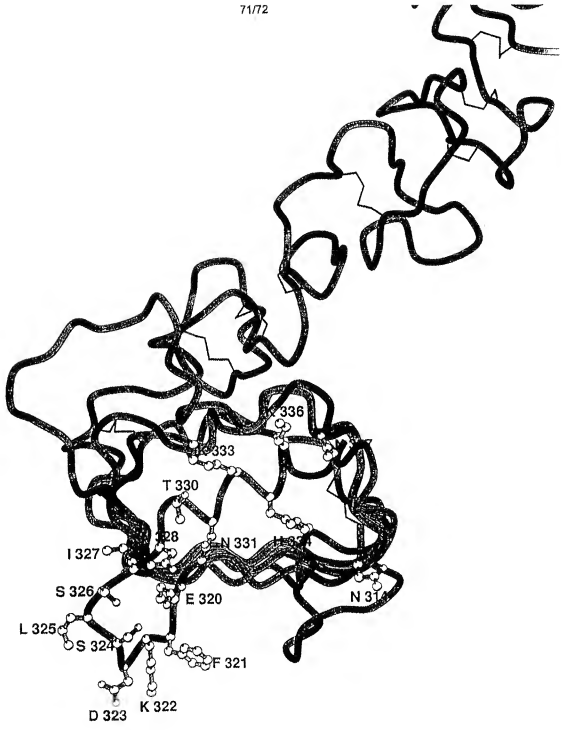
336
333
T 330
328
N 331
I 327
S 326
E 320
N 31
L 325
S 324
F 321
D 323
K 322

Figure 9

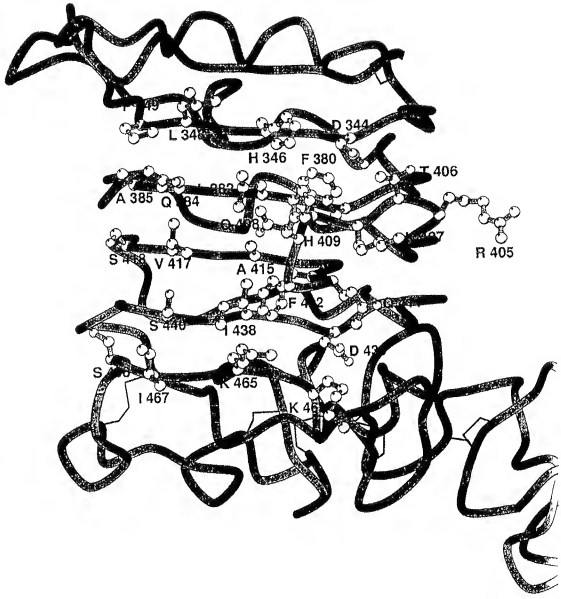
D 344
H 346
F 380
T 406
A 385
H 409
R 405
V 417
A 415
S 440
I 438
I 467
R 465

Figure 10

INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU 99/00420

A. CLASSIFICATION OF SUBJECT MATTER

Int Cl[6]: C07K 14/705, 14/71 G06F 17/50, 19/00, 159:00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
STN medline, Wpids, CA } (EGF receptor or "epidermal growth factor receptor" or ERB) and (design or model) and (structure or crystal structure or crystallog or x-ray)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X Y	Abe, Y. et. al., "Disulphide bond structure of human epidermal growth factor receptor", The Journal of Biological Chemistry Vol. 273 No. 18 ,1 May 1998 pages 11150 - 11157, particularly page 11153 and figures 2 and 3	1-23, 30-53 24-29
X Y	Sternberg, M.J.E et al., "Modelling the ATP binding site of onocogene products, the epidermal growth factor receptor and related proteins", FEBS Vol 175 No. 2 (October1984) pages 387-392	1-23, 30-53 24-29

[X] Further documents are listed in the continuation of Box C

[X] See patent family annex

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
20 July 1999	- 3 AUG 1999
Name and mailing address of the ISA/AU AUSTRALIAN PATENT OFFICE PO BOX 200 WODEN ACT 2606 AUSTRALIA Facsimile No.: (02) 6285 3929	Authorized officer K.F. PECK Telephone No.: (02) 6283 2263

Form PCT/ISA/210 (second sheet) (July 1998) GILLIAN JENKINS

INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU 99/00420

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
	Fry, D.W. et. al., "Design of a potent peptide inhibitor of the epidermal growth factor receptor tyrosine kinase utilizing sequences based on the natural phosphorylation sites of phospholipase C-γ1" Peptides Vol 15. No. 6 (1994)	
X	pages 951-957	1-23, 30-53
Y		24-29
	US, A 5708156 (Ilekis, J.V) published 13 January 1998	
X	see columns 1-5	1-23, 30-53
Y		24-29
	Garrett, T.P.J et al "Crystal structure of the first three domains of the type-1 insulin-like growth factor receptor "Nature Vol 394 published 23 July 1998	
X	pages 395-399	1-23, 30-53
Y		24-29
	WO, A, 94/25860 (Immunex Corporation) published 10 November 1994	
Y	see whole document	24-29

INTERNATIONAL SEARCH REPORT

International application No.
PCT/AU 99/00420

Box 1 Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☒ Claims Nos.: **36 to 53**
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

Please see supplemental box

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a)

Box II Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest
☐ The additional search fees were accompanied by the applicant's protest.
☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

international application No.
PCT/AU 99/00420

Box I

Claims 36-53 have no clear meaning. Claims 36-53 define compounds, pharmaceutical compositions and a method of use of the compound thereof obtained by the methods of any of claims 1 to 35. However claims 1 to 35 are directed to a method of designing compounds which bind to a molecule of the EGF receptor family based on the 3-D coordinates of the EGF receptor and not a method of preparing such compounds. Thus claims 36-53 merely identify a further property of the potential compound, that is that the compound may be obtained by the methods of claims 1 to 35. When the database used in the methods of claims 1 to 35 comprises chemical structures of known compounds, the compounds per se are not novel. Therefore claims 36, and 42-53 include known compounds (such as natural ligand EGF receptor and many synthetic EGF receptor analogs), that could have been obtained through means which do not involve the identification methods of claims 1 to 35. When the database used comprises virtual compounds, claims 36-53 do not have a clear meaning since the compounds are not real and may not exist. The specification has not described any compound that had been identified by the method of claims 1-35. Without specific examples that substantiate claims 36 to 53, the scope of these claims cannot be determined. Hence no meaningful search can be carried out.

Further to this any compound identified by the method of claims 1-35 may not be biologically active due to the unpredictable conditions experienced in-vivo.

INTERNATIONAL SEARCH REPORT
Information on patent family members

International application No.
PCT/AU 99/00420

This Annex lists the known "A" publication level patent family members relating to the patent documents cited in the above-mentioned international search report. The Australian Patent Office is in no way liable for these particulars which are merely given for the purpose of information.

Patent Document Cited in Search Report		Patent Family Member					
WO	94/25860	AU	67799/94	US	5453937	US	5557535
		US	5884230	AU	33037/97	WO	97/48060

END OF ANNEX